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## Multigroup neutron transport theory in plane geometry

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MULTIGROUP NEUTRON TRANSPORT THEORY  
IN PLANE GEOMETRY

by

B.E. CLANCY

Ph.D. Thesis

October 1970.





This thesis is submitted for the degree of  
Doctor of Philosophy to the Wollongong University College in  
the University of New South Wales, and has not been submitted  
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October 1970.

ABSTRACT

The multigroup form of the transport equation describing the steady state population of neutrons in a plane geometry is studied. The existing techniques of finding numerical solutions to the transport equation in the discrete ordinate approximation are considered in relation to the deep penetration problem of reactor shielding theory. Some of the computational difficulties are examined and a major one found to be the excessive time used in iterating the equation over a large number of mesh points.

A review is given of Chandrasekhar's reflection function method for finding solutions to an astrophysical problem equivalent to the one group form of the deep penetration problem in finite and semi infinite homogeneous media. After generalising the method it is shown how accurate solutions may be obtained for realistic multigroup problems in semi infinite media without the need for spatial iterations.

For many deep penetration problems in finite heterogeneous slabs only certain integrals of the angular neutron fluxes emerging from the slabs are of interest. A variational principle is devised with the aid of which solutions to appropriately chosen semi infinite medium problems can be used to calculate directly approximations to any integral of these emerging angular fluxes. From the results obtained with a computer programme embodying these methods it is found that significant savings in computing time can be achieved

when a number of survey calculations need to be performed.

Some possible applications of the reflection function method to other problems in neutron transport theory are examined briefly.

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## 1. INTRODUCTION

This thesis is concerned essentially with a particular neutron transport problem - that of calculating the way in which neutrons are transmitted through or reflected from large plane slabs. The problem arises when it is desired to assess the effectiveness of biological shields for power reactors and experimental assemblies. It can also arise in the design of experiments in which slabs of material are placed between a neutron source and the experimental rig in such a way as to modify the effective source in some way.

Over the years a variety of techniques have been used in attempting solutions of this deep penetration problem, techniques such as the moments method, diffusion theory and removal diffusion theory, collision probability methods, and methods based on expansion of the angular flux such as  $P_N$  and double  $P_N$  methods. A brief review of all these methods is given by Clifford, Mynatt and Straker (1969). For a variety of reasons none of these methods are considered in this study, which is restricted to the multigroup discrete ordinate (or discrete  $S_N$ ) treatment of the neutron transport equation (Wick, 1943; Chandrasekhar, 1944 and 1960; Carlson 1953). The  $S_N$  method is employed in many reactor physics computer codes such as WDSN (Green 1967), ANISN (Engle, 1967) and a host of older codes. All of these codes can be used to obtain approximate solutions to deep penetration problems and the basic features of the  $S_N$  method will now be described.

## 1.1 Discrete $S_N$ Codes

If the region of interest is free of fixed sources then the time independent multigroup transport equation in one dimensional slab geometry is

$$\sigma_g \phi_g(x, \mu) + \mu \frac{\partial \phi_g}{\partial x}(x, \mu) = \sum_{g'} \int_{-1}^1 \sigma(x; g', \mu' \rightarrow g, \mu) \phi_{g'}(x, \mu') d\mu' \quad (1.1)$$

$$= S_g(x, \mu).$$

In the discrete  $S_N$  codes this equation is solved for a discrete set of  $\mu$  values in the range  $(-1, 1)$ , the integration over  $\mu$  being computed by a quadrature formula. In equation (1.1) the notation is standard so that

$\sigma_g(x)$  is the group  $g$  total cross section at position  $x$ ,

$\phi_g(x, \mu) d\mu$  is the group  $g$  angular flux at  $x$  for the

interval  $\mu, \mu+d\mu$ ,

$\cos^{-1}(\mu)$  is the angle between the neutron direction and the positive  $x$  axis,

$\sigma(x; g', \mu' \rightarrow g, \mu)$  is the cross section at position  $x$  which

describes the rate of neutron transfers from group

$g'$  direction  $\mu'$  into group  $g$  direction  $\mu$ , so that

$S_g(x, \mu) d\mu dx$  is the number of neutrons per second being transferred into group  $g$  in the spatial interval  $x, x+dx$  with direction cosines between  $\mu$  and  $\mu+d\mu$ . The source term  $S_g(x, \mu)$  can in this formulation include transfers via the fission process as well as the scattering process.



In the codes the variation with  $x$  is treated by a finite difference approximation so that the angular fluxes are calculated at a set of discrete mesh points  $x_1, x_2, \dots, x_i, \dots, x_I$  between any two of which the material is taken as homogeneous. If equation (1.1) is integrated over the mesh interval  $x_i, x_{i+1}$ , it becomes for the discrete direction  $\mu_m$

$$\sigma_g \Delta \bar{\phi}_g(x_i, \mu_m) + \mu_m [\phi_g(x_{i+1}, \mu_m) - \phi_g(x_i, \mu_m)] = \Delta \bar{S}_g(x_i, \mu_m) \quad (1.2)$$

where  $\Delta = x_{i+1} - x_i$ , and the bars  $\bar{\phantom{x}}$  above  $\phi_g$  and  $S_g$  denote some average value across the mesh interval. The codes then solve equation (1.2) iteratively. The evaluation of the average angular source  $\bar{S}_g$  will be discussed in a later section and for now it suffices to say that it is determined from the angular fluxes calculated during the previous iteration. With  $\mu_m$  positive the new angular fluxes  $\phi(x_i, \mu_m)$  are determined successively from equation (1.2) with  $i$  increasing, the starting flux  $\phi_g(x_1, \mu_m)$  being determined from a boundary condition at the face  $x = x_1$ . When  $\mu_m$  is negative the boundary condition at the face  $x = x_I$  gives the starting value for the angular fluxes which are then determined consecutively in the order  $i = I, I-1, I-2, \dots, 2, 1$ .

### 1.1.1 The Transfer Source Term $S_g(x, \mu)$

The now standard procedure for calculation of the term  $S_g(x, \mu)$  in equation (1.1) is the so called multitable procedure. If for the moment it is assumed that no fission transfers occur then it is possible to define a group to group differential scattering cross section  $\sigma_{gg'}(\cos \theta_0) \equiv \sigma_{gg'}(\mu_0)$  which for transfers from group  $g'$  to group  $g$  is explicitly a function of the scattering angle  $\theta_0$ . Expanding this as a series of Legendre polynomials in  $\mu_0$  gives

$$\sigma_{gg'}(\mu_0) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} \sigma_{gg'}^{\ell} P_{\ell}(\mu_0) \approx \sum_{\ell=0}^L \frac{2\ell+1}{2} \sigma_{gg'}^{\ell} P_{\ell}(\mu_0) \quad (1.3)$$

and in the  $S_N$  codes the data entries are the  $L + 1$  transfer matrices

$$\sigma_{gg'}^{\ell}, \quad \ell = 0, 1, \dots, L.$$

If the expansion is inserted into equation (1.1) and use is made of the addition theorem for Legendre polynomials the source term becomes simply

$$S_g(x, \mu) = \sum_{g'} \sum_{\ell=0}^L \frac{2\ell+1}{2} \sigma_{gg'}^{\ell} P_{\ell}(\mu) \int_{-1}^1 P_{\ell}(\mu') \phi_{g'}(x, \mu') d\mu'. \quad (1.4)$$

If fissionable material is present this source term has to be modified to include fission neutrons but this modification is only made to the  $\ell = 0$  term since the fission process is essentially isotropic.

Within a mesh interval the average angular source is calculated from equation (1.4) by replacing the angular flux in that equation by the average value chosen for the mesh interval.

Because of computer storage limitations, the order  $L$  of anisotropic scattering retained in equation (1.4) is usually kept quite low. Though this may mean that the approximation of the differential scattering cross section in equation (1.3) is a very poor one, the calculation of the source term from equation (1.4) may not be much in error because of the smoothing effect of the integral and summation operations.

An illustration of this effect is given in Figures (1.1) and (1.2). For groups  $g'$ ,  $g$  covering the lethargy intervals 4.0 to 4.25 and 4.25 to 4.5 respectively the exact cross section  $\sigma_{gg'}(\mu_0)$  for scattering by Deuterium was calculated as was the  $L = 3$  approximation. These are given in Figure (1.1) using arbitrary units for the cross sections. It is clear that the agreement at this stage is poor. An angular flux in group  $g'$  was then selected rather arbitrarily as

$$\begin{aligned}\phi_{g'}(\mu) &= e^{-1/\mu} & 0 \leq \mu \leq 1 \\ &= 0 & -1 \leq \mu \leq 0\end{aligned}$$

and the contribution this makes to the angular source in group  $g$  calculated using the correct differential cross section and using

FIGURE 1.1

SIGMA(MU)

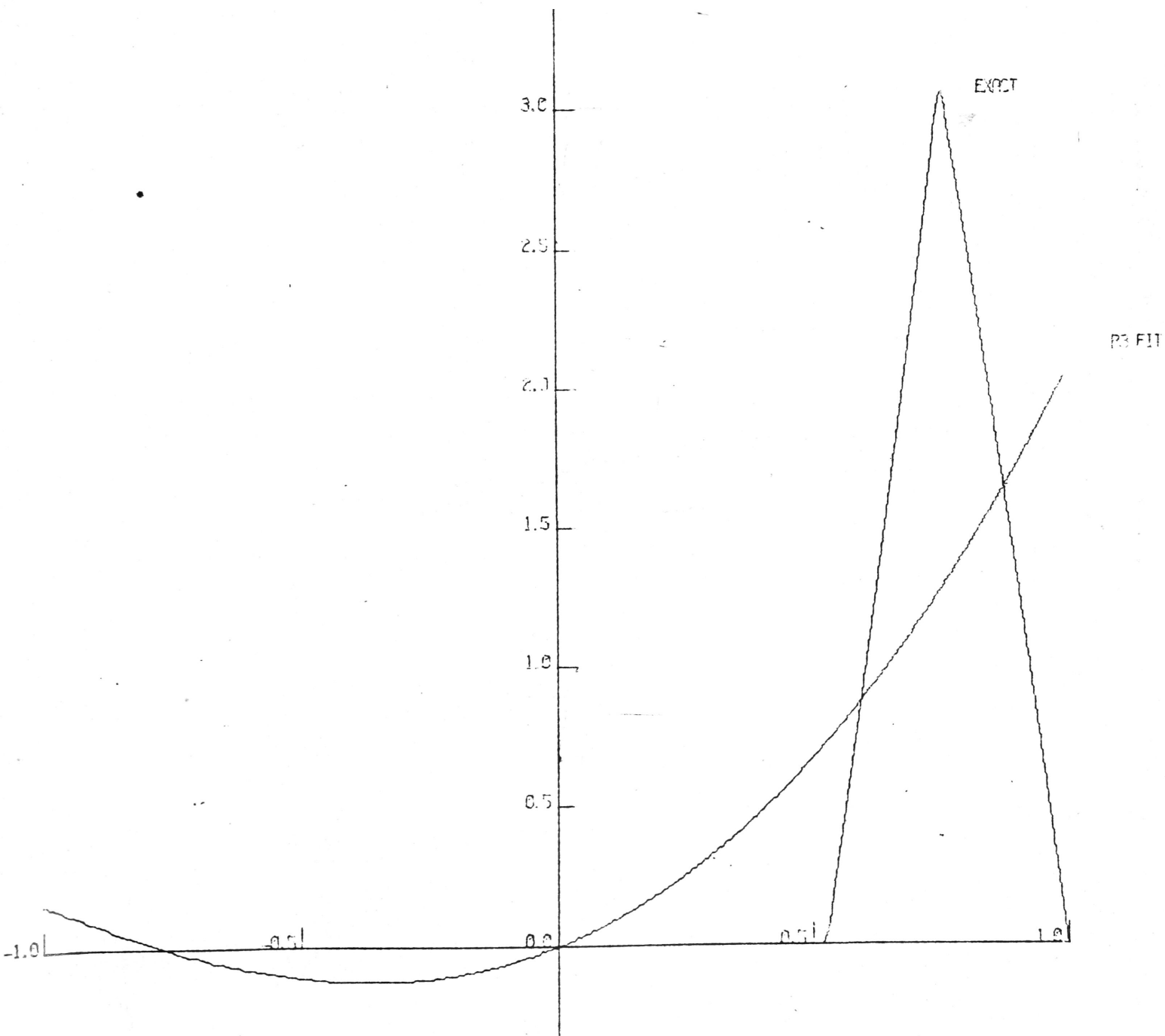
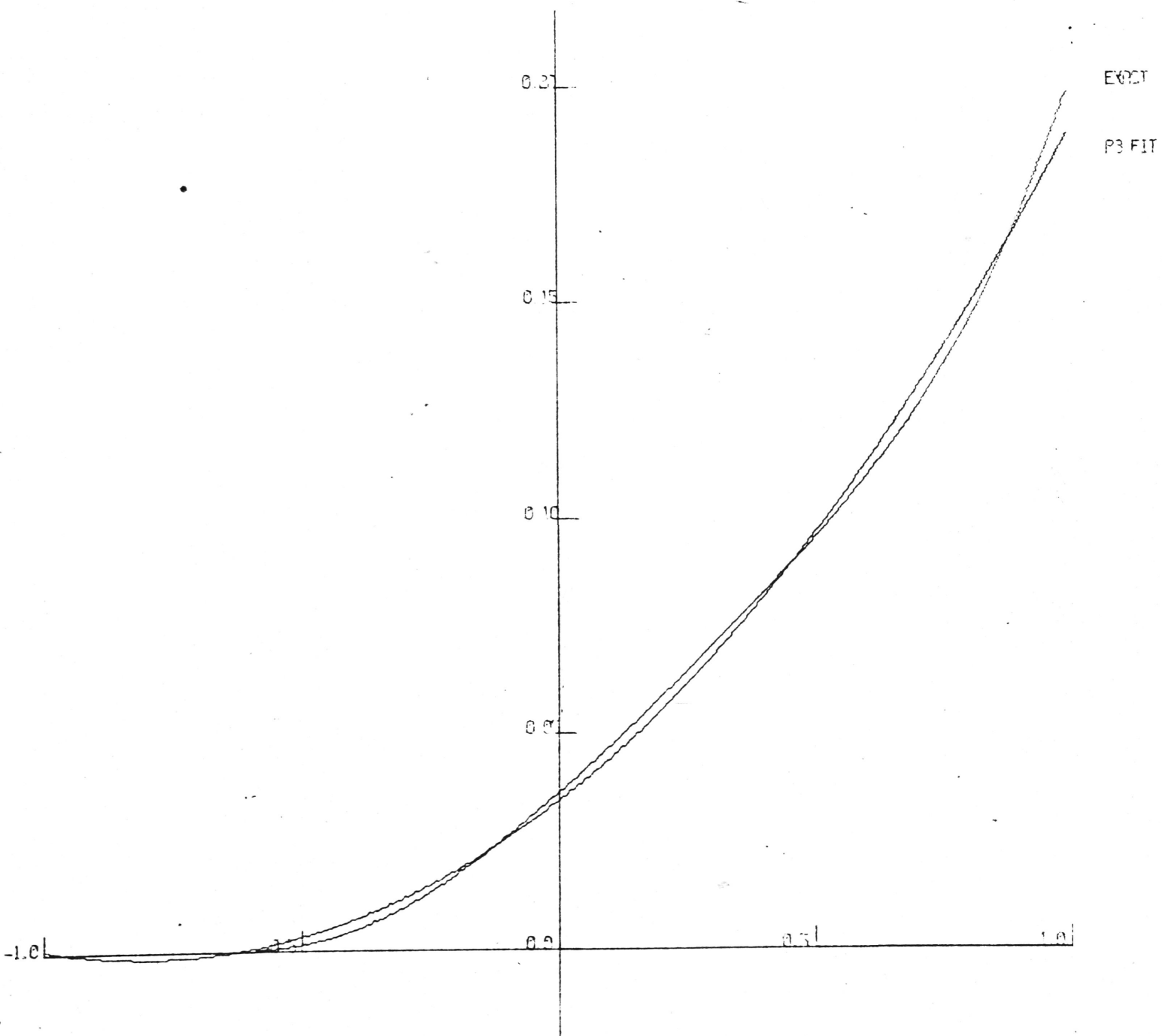


FIGURE 1.2

SOURCE(MU)



the  $L = 3$  approximation. These two angular source terms are shown in Figure (1.2). The adequacy of the approximation is surprisingly good, though it has the irritating defect of predicting a negative (and thus non physical) value for the source in the neighbourhood of  $\mu = -.75$ .

If the angular fluxes are nearly isotropic even lower values for  $L$  will be satisfactory and in many calculations the isotropic scattering assumption is employed with  $L = 0$ . This is very often modified by using some form of "transport approximation" in which an attempt is made to allow for anisotropy of the transfers while still retaining the simplicity and speed of the isotropic scattering approximation.

In deep penetration studies the group fluxes are far from isotropic and the anisotropy has to be included explicitly in calculations. For shielding studies third order ( $L = 3$ ) calculations seem to be necessary and are probably adequate.

The calculation of the set of transfer matrices  $\sigma_{ij}^0, \sigma_{ij}^1, \sigma_{ij}^2 \dots$  by averaging point cross section data over some appropriate spectrum is a routine data preparation task, and will not be discussed here.

### 1.1.2 Determination of Average Angular Fluxes

A problem which immediately arises is of defining the average angular flux  $\bar{\phi}_g(x_1, \mu_m)$ . The simplest definition is the linear average

$$\bar{\phi}_g(x_i, \mu_m) = \frac{1}{2}[\phi_g(x_i, \mu_m) + \phi_g(x_{i+1}, \mu_m)] \quad (1.5)$$

used invariably in WDSN but with some provisos in ANISN and the other American codes. With this definition it follows immediately from equation (1.2) that

$$\phi_g(x_{i+1}, \mu_m) = \frac{2\Delta\bar{S}_g + (2\mu_m - \Delta\sigma_g)\phi_g(x_i, \mu_m)}{2\mu_m + \Delta\sigma_g} \quad (1.6)$$

Unfortunately if the product  $\Delta\sigma_g$  is large this formula can produce a negative answer for the angular flux, which is not physically meaningful and indicates that the mesh interval is too large. In the American codes a standard practice is to trap these negative fluxes and to recompute them using a different definition for the average angular flux  $\bar{\phi}_g(x_i, \mu_m)$ . The usual "negative flux fixups" are however only a stopgap procedure and really accurate solutions for the angular fluxes cannot be achieved if they have been used. A detailed discussion of the difficulty is given by Mynatt et.al. (1969) who give explicit examples of the errors resulting when the standard fixup procedures are used in deep penetration problems. To guarantee positivity of all angular fluxes in a realistic shielding calculation many hundreds of mesh intervals may have to be used with a large penalty in computing time.

### 1.1.3 Solution by Iteration

Equations (1.2) to (1.5) with the boundary conditions on the angular fluxes are in the standard  $S_N$  codes solved iteratively.

One set of iterations called, in the jargon, the inner iteration loop, is concerned with the evaluation of the angular fluxes in a particular group and assumes the angular fluxes in other groups are fixed, so that the transfer sources into the group being solved are also fixed.

The second or outer iteration loop comprises a sweep through all of the groups, one inner iteration loop for each group. Usually the groups are solved consecutively starting with the highest energy group and finishing with the lowest energy group but the Mark I version of the code WDSN departed from this practice.

Like all iterative processes both these iteration loops may on occasions be irritatingly slow to converge and the processes may need to be accelerated.

For the inner iterations, where the spatial variation of the fluxes within one group are being computed, the most commonly used acceleration technique is the scaling method of Carlson and Bell (1958) or some variant of it. This method makes the assumption that after a particular inner iteration the fluxes have essentially the correct spatial shape but need to be multiplied by a constant



scale factor. The scale factor is estimated from the change in the scalar fluxes during the inner iteration. The technique was modified by Engle and Mynatt (1968) because of its poor performance for deep penetration problems where the fundamental assumption (that the flux shape is roughly correct after an inner iteration) breaks down. Engle and Mynatt showed how a separate scale factor could be calculated for each mesh point, and the application of their technique does make for rapid convergence in many problems, being more successful than the Chebechev acceleration techniques which they also investigated.

For the outer iteration loop no acceleration is needed for problems in which the transfer cross section matrices are triangular - which is so if the groups have been chosen so that no upscattering is possible and no fissionable materials are present.

If, however, these conditions are not satisfied then acceleration of the outer iteration loop may be necessary. Clancy and Donnelly (1970) described a method for calculation of a set of scale factors (one for each group) which materially improve the convergence rate for problems characterised by significant upscattering cross sections.

#### 1.1.4 Reduction of Mesh Points

At the end of section 1.1.2 it was mentioned that with the traditional discrete ordinate codes it may be necessary to use several hundreds of mesh intervals in a thick slab if accurate

answers are required for transmissions through the slab. The main reason for this is that the spatial variation of angular flux through a mesh interval is assumed in the codes to be linear. A major reduction in the number of mesh intervals required can be achieved if this unnecessarily simple assumption is abandoned.

If the angular source term  $S_g(x, \mu)$  is assumed known then equation (1.1) is a first order linear differential equation and its analytic solution is simple. For  $\mu$  positive the solution relates the angular fluxes on each side of a mesh interval  $(x_i, x_{i+1})$  of width  $\Delta$  by the equation

$$e^{\sigma_g \Delta / \mu} \phi(x_{i+1}, \mu) = \phi(x_i, \mu) + \frac{1}{\mu} \int_{x_i}^{x_{i+1}} e^{\sigma_g (x' - x_i) / \mu} S_g(x', \mu) dx'$$

with which no difficulties about negative fluxes can arise when the angular source  $S_g$  is positive. Some simple manipulations then make it possible to calculate exactly the average angular flux in the mesh interval. An assumption still has to be made about the spatial shape of the angular source term  $S_g(x, \mu)$  within the mesh interval and it has been found adequate to assume that this variation is linear with  $x$ . Full details of the method are given by Clancy (1969b) in a report describing a computer code written to explore the usefulness of the method.

## 1.2 The Need for Iterations

Even with a major reduction in the number of mesh intervals, *with* the acceleration techniques available the need for iteration over space points still is a major nuisance and, of course, the thicker the slab the greater the nuisance. This was first borne in on the candidate when faced with the problem of calculating the spectrum of neutrons returned to ground by the atmosphere - essentially a semi-infinite medium. Even though this is approximated by a large but finite slab it does conjure up the frightening vision of a never ending inner iteration loop. This problem not only brought home to the candidate the need for an alternative method of calculation for thick slabs, but also by its semi-infinite character suggested the method which is explored in the body of this thesis.

## 1.3 Layout of Succeeding Chapters

In Chapter 2 the method developed by Chandrasekhar for study of radiative transfer in semi-infinite atmospheres is discussed. Little if any of the material in this chapter is original but the results of Chandrasekhar and other workers are presented with a consistent notation and in the context of one group neutron transport theory.

In Chapter 3 Chandrasekhar's method for finite slabs is discussed, again in the context of one group neutron transport. The candidate's contribution in this chapter is the use of a

variational principle to derive, for Chandrasekhar's functions, approximations suitable for use with thick slabs.

In Chapter 4 Chandrasekhar's method for a semi-infinite medium is generalised so that multigroup transport problems with anisotropic group to group transfers can be treated. Originality was to have been claimed for this extension until August 1969 when to his chagrin the candidate read the paper of Pahor and Shultis (1969) which anticipated this extension. Their work was, however, restricted to the isotropic transfer approximation and originality is still claimed for the anisotropic transfer treatment and for the material of Chapters 5 and 6.

In Chapter 5 the multigroup analysis is combined with a variational principle to give a method for calculating neutron transmissions through (and reflections from) large finite slabs.

Finally in Chapter 6 some additional applications of Chandrasekhar's method to neutron transport problems are explored briefly.

## 2. ONE GROUP THEORY FOR A SEMI INFINITE MEDIUM

In this chapter we introduce the method of Chandrasekhar in its simplest form and apply it to some one group transport problems in a semi infinite medium. Most of this analysis has been performed by earlier workers in differing notations but is repeated here for completeness and consistency. Where possible, the treatment of Auerbach (1961) is followed, particularly in the solution of the albedo and Milne problems discussed in section 2.3. The Milne problem with absorption will be treated in rather more detail than the other problems, because Auerbach only discussed this problem in the absorption free case. We believe our treatment of this problem is simpler than the Wiener Hopf treatment used for example by Case, de Hoffman and Placzek (1953), with whose results complete agreement is obtained.

### 2.1 Chandrasekhar's Method for Isotropic Scattering

For a homogeneous isotropically scattering semi infinite medium in which one energy group theory is applicable the plane geometry transport equation may be written

$$\phi(x, \mu) + \mu \frac{\partial}{\partial x} \phi(x, \mu) = Q(x, \mu) + \frac{c}{2} \int_{-1}^1 \phi(x, \mu') d\mu' \quad (2.1)$$

for  $0 \leq x \leq \infty$  and  $-1 \leq \mu \leq 1$ . Here the variable  $x$  measures distances into the slab from the face  $x = 0$  in units chosen to make the total cross section unity. The parameter  $c$ , restricted

to the range  $0 \leq c \leq 1$ , denotes the average number of secondary neutrons produced on a collision, whilst  $\phi(x, \mu)$  and  $Q(x, \mu)$  are respectively the angular flux and angular source within the medium. To specify a transport problem completely conditions must be imposed on the angular flux both at the boundary  $x = 0$  and as  $x$  tends to  $\infty$ .

The Chandrasekhar method begins by dividing the angular flux into two components  $\phi(x, +\mu)$  and  $\phi(x, -\mu)$ , where the first function describes neutrons moving towards the right, and the second function describes neutrons moving towards the left. A reflection function  $(1/2\mu)S(\mu, \mu')$ ,  $0 < \mu, \mu' \leq 1$  independent of  $x$  is then defined such that the flux at  $x$  in direction  $-\mu$  is given by

$$\phi(x, -\mu) = \phi_x(x, -\mu) + \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \phi(x, +\mu') d\mu'. \quad (2.2)$$

The function  $\phi_x(x, -\mu)$  represents neutrons originating in the medium to the right of  $x$  and crossing the  $x$ -plane for the first time. Since the distribution of these neutrons is independent of the presence of material and sources to the left of  $x$ ,  $\phi_x(x, -\mu)$  is the left going flux which would exist at  $x$  as a result of volume sources if all the material to the left of  $x$  were removed. The second term on the right hand side of equation (2.2) represents those neutrons moving towards the left as a result of having crossed the  $x$ -plane in a direction  $+\mu'$  and having been reflected back into the direction  $-\mu$  by the material behind  $x$ .

The function  $\phi_x(x, -\mu)$  was introduced by Horak (1952) whilst the use of the reflection function was originated by Ambarzumian (1942, 1943) whose work was amplified and extended by Chandrasekhar (1960) and by Busbridge (1960). No matter where the x-plane is drawn there is always a semi infinite medium to the right of it and the scattering function  $S(\mu, \mu')$  is thus independent of x as well as of the sources. An equation for the function  $S(\mu, \mu')$  can now be derived by considering the pair of equations (2.1) and (2.2) in the absence of volume sources and with boundary conditions

$$\phi(0, \mu) = \delta(\mu - \mu_0), \quad 0 < \mu, \quad \mu_0 \leq 1 \quad (2.3)$$

$\lim_{x \rightarrow \infty} \phi(x, \mu)$  remains finite.

Physically this corresponds to a monodirectional beam of neutrons impinging onto the medium at the surface  $x = 0$ . With no volume sources the terms  $Q(x, \mu)$  in equation (2.1) and  $\phi_x(x, -\mu)$  in equation (2.2) vanish. Differentiating equation (2.2) with respect to x and setting  $x = 0$  gives

$$\dot{\phi}(0, -\mu) = \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \dot{\phi}(0, +\mu') d\mu' \quad (2.4)$$

and on the surface of the slab

$$\phi(0, -\mu) = \frac{1}{2\mu} S(\mu, \mu_0). \quad (2.5)$$

The derivatives of the angular flux at  $x = 0$  can be found from equation (2.1) which is written

$$\begin{aligned} \dot{\phi}(0, \pm\mu) = & \mp \frac{1}{\mu} \phi(0, \pm\mu) \pm \frac{c}{2\mu} \int_0^1 \phi(0, \mu') d\mu' \\ & \pm \frac{c}{2\mu} \int_0^1 \phi(0, -\mu') d\mu'. \end{aligned} \quad (2.6)$$

Substituting (2.3) and (2.5) into (2.6) gives an explicit form for the derivatives and when these are inserted into (2.4) there results after some re-arrangement

$$\left(\frac{1}{\mu} + \frac{1}{\mu_0}\right) S(\mu, \mu_0) = c \left(1 + \int_0^1 S(\mu, \mu') \frac{d\mu'}{2\mu'}\right) \left(1 + \int_0^1 S(\mu'', \mu_0) \frac{d\mu''}{2\mu''}\right). \quad (2.7)$$

Now the optical reciprocity theorem of Case, de Hoffman and Placzek (1953) implies that  $S$  is symmetric, i.e. that  $S(\mu, \mu_0) = S(\mu_0, \mu)$ . The square bracketed terms in equation (2.7) then have the same functional form and each is defined as the isotropic scattering Chandrasekhar  $H$ -function so that

$$H(\mu) = 1 + \int_0^1 S(\mu, \mu') \frac{d\mu'}{2\mu'}. \quad (2.8)$$

Equations (2.7) and (2.8) then become

$$S(\mu, \mu_0) = \frac{c\mu\mu_0}{\mu + \mu_0} H(\mu)H(\mu_0) \quad (2.9)$$

$$H(\mu) = 1 + \frac{c}{2\mu} H(\mu) \int_0^1 \frac{H(\mu')}{\mu + \mu'} d\mu'. \quad (2.10)$$



Chandrasekhar (1960) has shown that the function  $H(\mu)$  may be expressed in the form of a definite integral

$$H(\mu) = \exp \left\{ -\frac{\mu}{\pi} \int_0^{\pi/2} \frac{\log(1 - c\theta \cot \theta)}{\cos^2 \theta + \mu^2 \sin^2 \theta} d\theta \right\} \quad (2.11)$$

but numerical values of  $H(\mu)$  are most easily found for  $0 \leq \mu \leq 1$  by iterating equation (2.10). This was the method used by Chandrasekhar (1960) who first tabulated the function. More rapid convergence is obtained by casting equation (2.10) in the form

$$H(\mu) = \left( 1 - \frac{c}{2} \mu \int_0^1 \frac{H(\mu')}{\mu + \mu'} d\mu' \right)^{-1} \quad (2.12)$$

and iterating this form instead. Convergence is slowest when  $c \approx 1$  and Shure and Natelson (1964) have derived an alternative form which converges more rapidly in this range. For general purposes however, equation (2.12) is satisfactory enough.

Equations (2.10) and (2.12) admit of two solutions, the function  $H(\mu)$  defined by equation (2.11) and a second solution  $(1 + \kappa\mu)H(\mu)/(1 - \kappa\mu)$  where  $\kappa$  (the inverse diffusion length) is the positive root of

$$\kappa = \frac{c}{2} \log \left( \frac{1+\kappa}{1-\kappa} \right). \quad (2.13)$$

However the three iteration procedures mentioned are all known (Noble 1964) to converge to the required solution (2.11) with reasonable zero-th iterates. In numerical work carried out by the candidate these zero-th iterates were always chosen so as to

make their integral over the range (0,1) have the correct value.

## 2.2 Properties of the Isotropic Scattering H-Function

### 2.2.1 Moments of $H(\mu)$

If the moments  $h_n$  are defined

$$h_n = \int_0^1 \mu^n H(\mu) d\mu,$$

then they are found to satisfy the relationship

$$h_{2n} = \frac{1}{2n+1} + \frac{c}{4} \sum_{j=0}^{2n} (-)^j h_{2n-j} h_j. \quad (2.14)$$

To prove this equation (2.10) is multiplied through by  $\mu^{2n}$  and integrated over the range  $0 \leq \mu \leq 1$  giving

$$h_{2n} = \frac{1}{2n+1} + \frac{c}{2} \int_0^1 H(\mu) d\mu \int_0^1 \frac{\mu^{2n+1}}{\mu+\mu'} H(\mu') d\mu'.$$

By repeated division we can write

$$\frac{\mu^{2n+1}}{\mu+\mu'} = \sum_{j=0}^{2n} (-)^j \mu^{2n-j} (\mu')^j - \frac{(\mu')^{2n+1}}{\mu+\mu'}$$

from which it follows that

$$h_{2n} = \frac{1}{2n+1} + \frac{c}{2} \sum_{j=0}^{2n} (-)^j h_{2n-j} h_j - \frac{c}{2} \int_0^1 H(\mu) d\mu \int_0^1 \frac{(\mu')^{2n+1}}{\mu+\mu'} H(\mu') d\mu'.$$

Elimination of the double integral between the two equations for  $h_{2n}$  then gives equation (2.14) directly.

For  $n = 0$  equation (2.14) becomes a quadratic equation for  $h_0$  with roots

$$h_0 = \frac{2}{c}(1 \pm \sqrt{1-c}).$$

The smaller root applies to the smaller solution of equation (2.10) so that

$$\int_0^1 H(\mu) d\mu = h_0 = \frac{2}{c}(1 - \sqrt{1-c})$$

and for  $c = 1$  (i.e. the case of zero absorption) this reduces to

$$h_0 = 2.$$

For  $c = 1$  when  $n = 1$  is substituted into equation (2.14) the terms involving  $h_2$  drop out and we find

$$h_1 = 2/\sqrt{3}$$

but no such simple result holds for  $c < 1$ .

### 2.2.2 $H(z)$ as a function of a complex variable

With  $H(\mu)$  defined for  $0 \leq \mu \leq 1$  equations (2.10) or (2.12) may be used to extend the domain of definition of the H-function to the complex plane, so that

$$H(z) = \left( 1 - \frac{c}{2} z \int_0^1 \frac{H(\mu')}{z + \mu'} d\mu' \right)^{-1} \quad (2.17)$$

for  $z$  in the complex plane cut along the real interval

$-1 \leq z \leq 0$ . With  $H(z)$  defined in this way it is possible to

develop in an elementary way a relation of some utility for later analysis. From equation (2.17) we have for  $z \notin (-1,1)$

$$\begin{aligned} \left(\frac{1}{H(z)} - 1\right) \left(\frac{1}{H(-z)} - 1\right) &= \frac{c^2}{4} z^2 \int_0^1 \frac{H(\mu')}{z+\mu'} d\mu' \int_0^1 \frac{H(\mu'')}{z-\mu''} d\mu'' \\ &= \frac{c^2}{4} z \int_0^1 H(\mu') d\mu' \int_0^1 H(\mu'') d\mu'' \left\{ \frac{\mu'}{z+\mu'} + \frac{\mu''}{z-\mu''} \right\} \frac{1}{\mu' + \mu''} \end{aligned}$$

after a partial fraction expansion. This right hand side can be written

$$\begin{aligned} &= \frac{c}{2} z \int_0^1 \frac{c}{2} \mu' H(\mu') \frac{d\mu'}{z+\mu'} \int_0^1 H(\mu'') \frac{d\mu''}{\mu' + \mu''} \\ &+ \frac{c}{2} z \int_0^1 \frac{c}{2} \mu'' H(\mu'') \frac{d\mu''}{z-\mu''} \int_0^1 H(\mu') \frac{d\mu'}{\mu' + \mu''} \\ &= \frac{c}{2} z \int_0^1 \frac{H(\mu')-1}{z+\mu''} d\mu' + \frac{c}{2} z \int_0^1 \frac{H(\mu'')-1}{z-\mu''} d\mu'' \\ &= \left(\frac{1}{H(z)} - 1\right) - \frac{c}{2} z \int_0^1 \frac{d\mu'}{z+\mu'} + \left(\frac{1}{H(-z)} - 1\right) - \frac{c}{2} z \int_0^1 \frac{d\mu''}{z-\mu''} \end{aligned}$$

by repeated application of equation (2.10). After the two integrations are performed and the resulting equation simplified there emerges the result sought, that

$$H(z)H(-z)T(z) = 1 \quad (2.18)$$

with

$$T(z) = 1 - \frac{c}{2} z \log \left| \frac{z+1}{z-1} \right|.$$

A more careful analysis shows however that the relation (2.18) holds over the whole complex plane (see for example Pahor and Zweifel (1969)).

The zeroes of  $T(z)$  thus determine the poles of  $H(z)$  and these are discussed by Bushbridge (1960). We simply remark that for  $0 < c < 1$  these zeroes are at  $z = \pm \frac{1}{\kappa}$  where the inverse relaxation length  $\kappa$  is defined by equation (2.13) and that  $H(z)$  has a simple pole at  $z = -\frac{1}{\kappa}$ . From equation (2.17) it then follows that

$$\int_0^1 \frac{H(\mu)}{1-\kappa\mu} d\mu = \frac{2}{c},$$

a result which is needed in proving that the second 'non-physical' solution of equation (2.10) is  $(1 + \kappa\mu)H(\mu)/(1 - \kappa\mu)$ . The physical solution has been computed for a range of values of  $c$  and for  $\mu > 0$  and is shown graphically in Figures 2.1 and 2.2.

### 2.3 Classical Transport Problems in One Group Theory

The properties of the  $H$ -function discussed in the previous section are sufficient for solution of some classical problems in transport theory. For most of these we follow the outline of Auerbach (1961) who seems to have been the first to apply Chandrasekhar's method to neutron transport problems, most of his work however being limited to models in which scattering was treated as isotropic in the laboratory system. Pahor (1966) used a combination of Chandrasekhar's method and the singular

FIGURE 2.1

$H(\mu) \nu \mu$ ,  $\mu = 0$  TO 1

$C = 0.2 ( 0.2 ) 1.0$

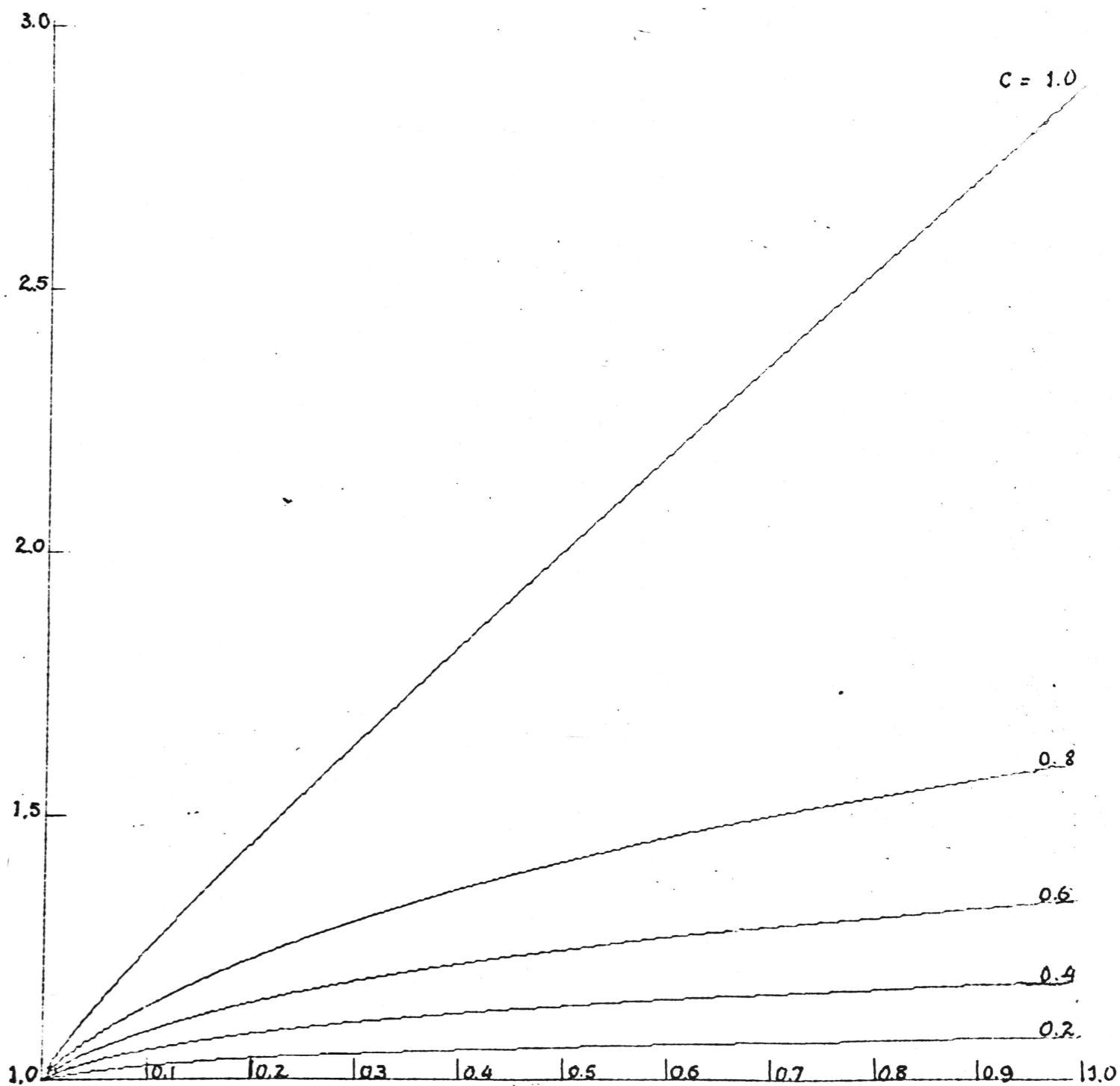
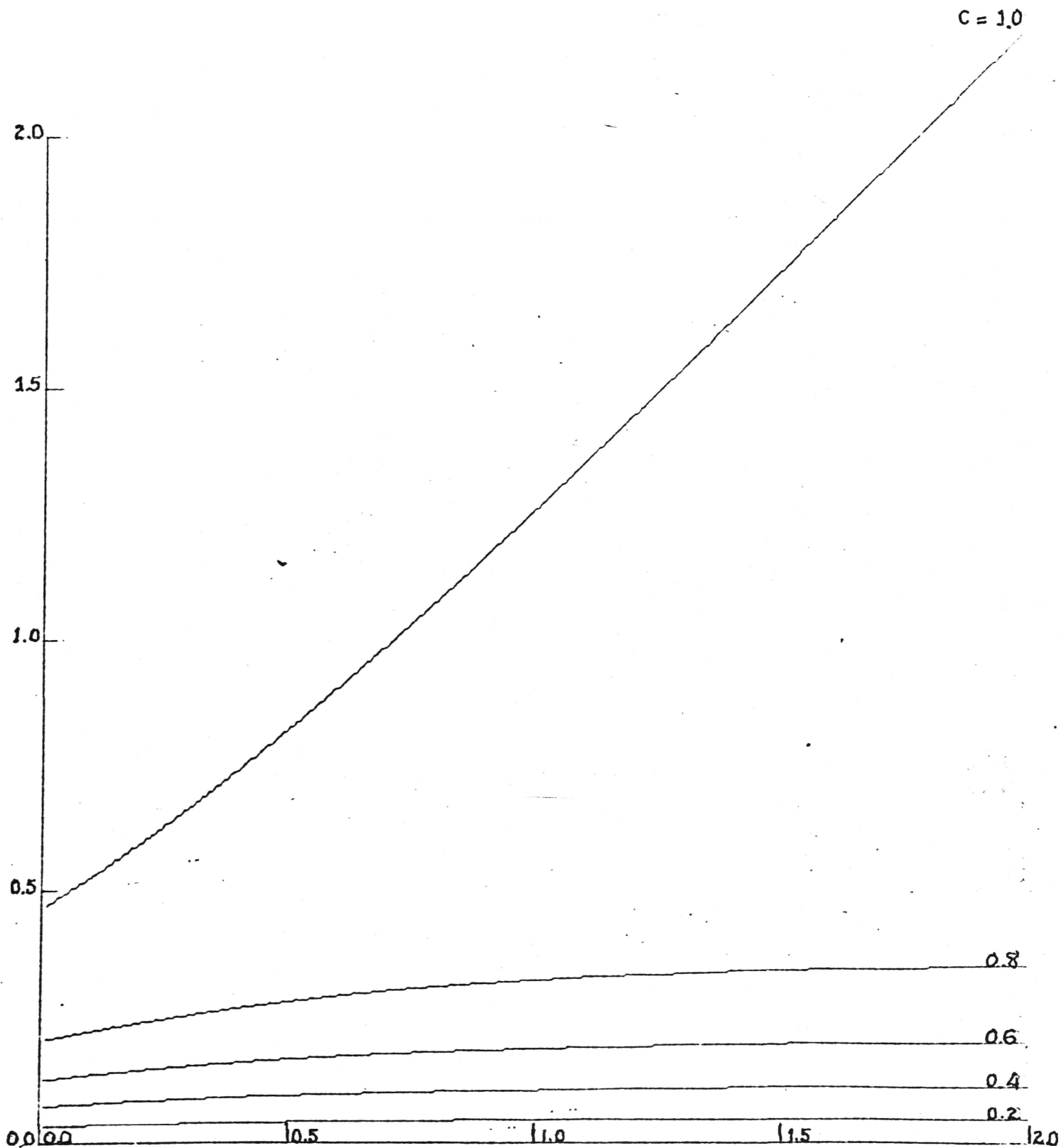


FIGURE 2.2

$\text{LOG}(H(\text{MU})) \sqrt{\text{LOG}(\text{MU})}$ ,  $\text{MU} = 1 \text{ TO } 100$

$C = 0.2 \text{ ( } 0.2 \text{ ) } 1.0$



eigen-function method of Case (1960) to treat these problems for general anisotropic scattering. The three problems to be discussed are

(i) evaluation of the particle current albedo  $A_2(\theta_0)$  for a semi infinite medium where  $A_2(\theta_0)$  is the ratio of reflected to incident currents when the incident angular flux is a mono-directional beam making an angle  $\theta_0$  with the normal to the slab.

(ii) The albedo problem - the determination of the neutron fluxes in the interior of the medium when a given angular flux impinges on the medium -

and (iii) the Milne problem, for which the neutron source in the medium is at infinity and the behaviour of the neutron fluxes near the boundary plane  $x = 0$  is of interest.

### 2.3.1 Evaluation of total particle current albedo $A_2(\theta_0)$

Following Selph (1968) we define

$$A_2(\theta_0) = \frac{\int_0^1 \mu \phi(0, -\mu) d\mu}{\int_0^1 \mu \phi(0, +\mu) d\mu} = \frac{J_-}{J_+} .$$



Here

$$\phi(0, \mu) = \delta(\mu - \mu_0), \quad \mu_0 = \cos \theta_0$$

so that

$$J_+ = \mu_0.$$

From equations (2.5) and (2.9)

$$\phi(0, -\mu) = \frac{c}{2} \frac{\mu_0}{\mu + \mu_0} H(\mu) H(\mu_0)$$

and

$$J_- = \frac{c}{2} \mu_0 H(\mu_0) \int_0^1 \frac{\mu H(\mu)}{\mu + \mu_0} d\mu$$

$$= \frac{c}{2} \mu_0 H(\mu_0) \left( \int_0^1 H(\mu) d\mu - \mu_0 \int \frac{H(\mu)}{\mu + \mu_0} d\mu \right).$$

From equations (2.15) and (2.10) it follows that

$$J_- = \mu_0 - \mu_0 H(\mu_0) \sqrt{1-c}$$

and finally

$$A_2(\theta_0) = 1 - H(\mu_0) \sqrt{1-c}$$

in conformity with the result of Spencer, Diaz and Moses (1964).

### 2.3.2 The albedo problem

Here a solution of the source free transport equation

$$\phi(x, \pm\mu) \pm \mu \frac{\partial}{\partial x} \phi(x, \pm\mu) = \frac{c}{2} \int_{-1}^1 \phi(x, \mu') d\mu' \quad (2.21)$$

is sought, with a prescribed value for  $\phi(0, \mu)$  when  $\mu$  is positive.

Because the linearity of the transport equation admits the superposition of solutions we need initially only seek the solution appropriate to the boundary conditions

$$\begin{aligned}\phi(0, \mu) &= \delta(\mu - \mu_0), \quad 0 < \mu, \mu_0 \leq 1 \\ \lim_{x \rightarrow \infty} \phi(x, \pm \mu) &= 0.\end{aligned}$$

With the reflection function defined by equations (2.5) and (2.9) the emerging angular fluxes are then simply

$$\phi(0, -\mu) = \frac{c}{2} \cdot \frac{\mu_0}{\mu + \mu_0} H(\mu) H(\mu_0)$$

and the complete knowledge of the initial angular fluxes makes feasible a solution of equation (2.21) by one sided Laplace Transform methods. The Laplace Transform of the angular flux  $\phi(x, \mu)$  is written as

$$\bar{\phi}(\rho, \mu) = \int_0^{\infty} e^{-\rho x} \phi(x, \mu) dx$$

and then

$$\bar{\phi}(\rho) = \int_0^{\infty} e^{-\rho x} \phi(x) dx = \int_{-1}^1 \bar{\phi}(\rho, \mu) d\mu$$

by reversing the order of the integrations.

The Laplace Transform of equation (2.21) is then

$$\bar{\phi}(\rho, \pm \mu) \pm \mu \rho \bar{\phi}(\rho, \pm \mu) \mp \mu \phi(0, \pm \mu) = \frac{c}{2} \bar{\phi}(\rho)$$

or

$$\bar{\phi}(\rho, \pm \mu) = \frac{\frac{c}{2} \bar{\phi}(\rho) \pm \mu \phi(0, \pm \mu)}{1 \pm \rho \mu}$$

and integration of this equation over  $\mu$  gives

$$\begin{aligned}
 \bar{\phi}(\rho) &= \int_0^1 \left\{ \bar{\phi}(\rho, +\mu) + \bar{\phi}(\rho, -\mu) \right\} d\mu \\
 &= \frac{c}{2} \bar{\phi}(\rho) \int_0^1 \frac{1}{1+\rho\mu} + \frac{1}{1-\rho\mu} d\mu \\
 &\quad + \int_0^1 \frac{\mu \delta(\mu - \mu_o)}{1+\rho\mu} d\mu \\
 &\quad - \frac{c}{2} \int_0^1 \frac{\mu \mu_o}{1-\rho\mu} \cdot \frac{H(\mu)H(\mu_o)}{\mu \cdot \mu_o} d\mu .
 \end{aligned}$$

The first two of these three integrals are elementary and the last yields to a partial fraction expansion and repeated application of equation (2.17). Thus

$$\begin{aligned}
 \bar{\phi}(\rho) &\left\{ 1 - \frac{c}{2\rho} \log \left( \frac{1+\rho}{1-\rho} \right) \right\} \\
 &= \int_0^1 \frac{\mu \delta(\mu - \mu_o)}{1+\rho\mu} d\mu - \frac{c}{2} \mu_o H(\mu_o) \int_0^1 \frac{\mu H(\mu)}{(1-\rho\mu)(\mu + \mu_o)} d\mu \\
 &= \frac{\mu_o}{1+\rho\mu_o} + \frac{c}{2} \frac{\mu_o H(\mu_o)}{1+\rho\mu_o} \left( \int_0^1 \frac{\mu_o H(\mu)}{\mu + \mu_o} d\mu + \int_0^1 \frac{H(\mu)}{\rho\mu - 1} d\mu \right) \\
 &= \frac{\mu_o}{1+\rho\mu_o} \left\{ 1 + \frac{c}{2} \mu_o H(\mu_o) \int_0^1 \frac{H(\mu)}{\mu + \mu_o} d\mu + \frac{c}{2} H(\mu_o) \int_0^1 \frac{H(\mu)}{\rho\mu - 1} d\mu \right\}
 \end{aligned}$$

$$\begin{aligned}
\bar{\phi}(\rho) & \left( 1 - \frac{c}{2\rho} \log \left( \frac{1+\rho}{1-\rho} \right) \right) \\
& = \frac{\mu_o}{1+\rho\mu_o} \left( H(\mu_o) + H(\mu_o) \frac{1-H(-1/\rho)}{H(-1/\rho)} \right) \\
& = \frac{\mu_o H(\mu_o)}{(1+\rho\mu_o) H(-1/\rho)}
\end{aligned}$$

and

$$\bar{\phi}(\rho) = \frac{\mu_o H(\mu_o)}{(1+\rho\mu_o) \left( 1 - \frac{c}{2\rho} \log \left| \frac{1+\rho}{1-\rho} \right| \right) H(-1/\rho)}, \quad (2.22)$$

or by application of equation (2.18)

$$\bar{\phi}(\rho) = \frac{\mu_o H(\mu_o) H(1/\rho)}{(1 + \rho\mu_o)} \quad , \quad \pm \rho \notin (1, \infty). \quad (2.23)$$

On physical grounds we can argue that for  $c \leq 1$  the scalar flux  $\phi(x)$  is bounded as  $x \rightarrow \infty$  and has a continuous derivative for  $x > 0$ . It follows from the theory of the Laplace Transform that  $\bar{\phi}(\rho)$  is regular in the half plane  $\text{Re}(\rho) > 0$  and that

$$\phi(x) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{\rho x} \bar{\phi}(\rho) d\rho$$

i.e.

$$\phi(x) = \frac{\mu_o H(\mu_o)}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{\rho x} d\rho}{(1+\rho\mu_o) \left( 1 - \frac{c}{2\rho} \log \frac{1+\rho}{1-\rho} \right) H(-1/\rho)}$$

where the path of integration is shown in Figure (2.3). The alternative expression (2.23) shows that the zero of

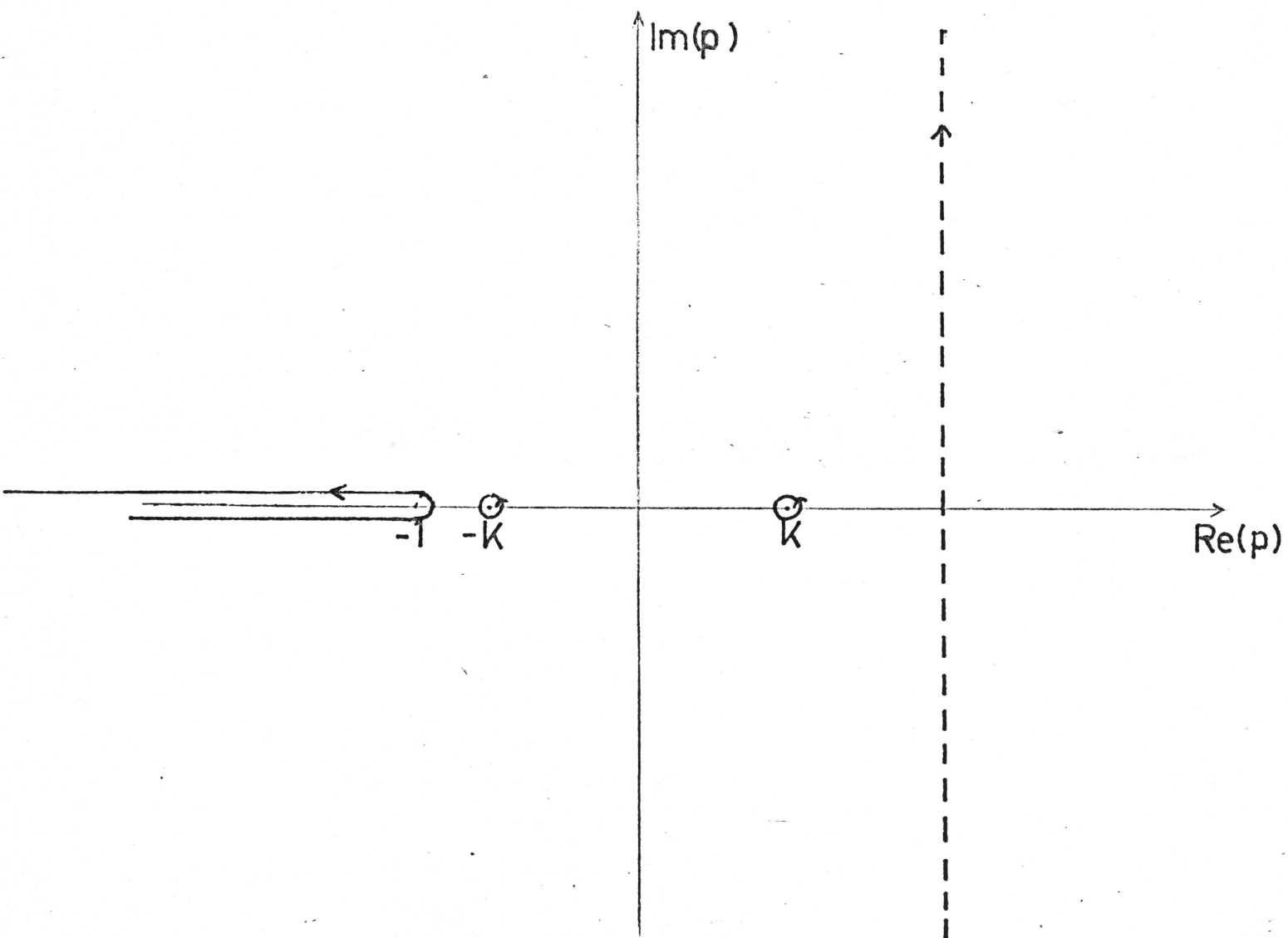
$$T(1/\rho) = 1 - \frac{c}{2\rho} \log \left| \frac{1+\rho}{1-\rho} \right| \quad \text{at } \rho = +\kappa$$

FIGURE 2.3

Contours for Transform Inversion

Original -----

Deformed \_\_\_\_\_



does not contribute anything to the inversion integral and the integration contour can be deformed to the alternative shape shown in Figure (2.3).

The asymptotic part of the solution comes from the integral around the pole at  $\rho = -\kappa$ , and from Cauchy's residue theorem this is

$$\phi_{\text{asy}}(x) = \frac{\mu_o H(\mu_o) e^{-\kappa x}}{(1-\kappa\mu_o) H(1/\kappa) \left( \frac{d}{d\rho} T(1/\rho) \right)_{\rho=-\kappa}}$$

or

$$\phi_{\text{asy}}(x) = \frac{\mu_o H(\mu_o) \kappa e^{-\kappa x}}{(1-\kappa\mu_o) H(1/\kappa) \left( \frac{c}{1-\kappa^2} - 1 \right)}.$$

Insertion of this result into the transport equation (2.21) gives the asymptotic form of the angular flux

$$\phi_{\text{asy}}(x, \mu) = \frac{c}{2(1-\kappa\mu)} \phi_{\text{asy}}(x).$$

The transient part of the solution is given by Auerbach (1961) who also discusses the necessary modification to equations (2.24) and (2.25) when  $c = 1$ .

### 2.3.3 The Milne problem

In this classical problem we are interested in the solution of the transport equation (2.1) with no inward flow of neutrons at  $x = 0$ . The neutrons in the half space  $x > 0$  are supplied by some source at  $x = \infty$ . This source will set up, as  $x \rightarrow \infty$ , an asymptotic spatial shape for the neutron distribution

of the form  $e^{\kappa x}$  where  $\kappa$  is the inverse relaxation length.

It is first necessary to find the angular distribution of neutrons leaving the face  $x = 0$ . To this end we note that with neutrons being born at infinity the term  $\phi_x(x, -\mu)$  in equation (2.2) is now no longer zero and must be evaluated. This is done from a physical argument by noting that  $\phi_x(x, -\mu)$  is the angular flux at  $x$  if all the material to the left of  $x$  is removed. Since this removal simply shifts the whole problem a distance  $x$  towards the source the  $x$  dependence of  $\phi_x(x, -\mu)$  is given also by an  $e^{\kappa x}$  form. Because there are no neutrons entering the medium at  $x = 0$

$$\phi_x(0, -\mu) = \phi(0, -\mu)$$

so that

$$\phi_x(x, -\mu) = e^{\kappa x} \phi(0, -\mu).$$

Equation (2.2) now becomes

$$\phi(x, -\mu) = e^{\kappa x} \phi(0, -\mu) + \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \phi(x, \mu') d\mu'$$

and after differentiating this equation with respect to  $x$  and setting  $x = 0$  we have

$$\dot{\phi}(0, -\mu) = \kappa \phi(0, -\mu) + \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \dot{\phi}(0, \mu') d\mu' . \quad (2.26)$$

The transport equation (2.21) evaluated at  $x = 0$  gives alternative forms for the spatial derivatives

$$\dot{\phi}(0, +\mu) = \frac{c}{2\mu} \int_0^1 \phi(0, -\mu') d\mu'$$

$$\dot{\phi}(0, -\mu) = \frac{1}{\mu} \phi(0, -\mu) - \frac{c}{2\mu} \int_0^1 \phi(0, -\mu') d\mu'$$

since  $\phi(0, \mu) = 0$ . (2.27)

If these expressions are substituted into equation (2.26)

and equation (2.9) is used for the reflection function

$S(\mu, \mu')$  we find

$$\frac{1}{\mu} \phi(0, -\mu) - \frac{c}{2\mu} A = \kappa \phi(0, -\mu) - \frac{c^2}{4} A H(\mu) \int_0^1 \frac{H(\mu')}{\mu + \mu'} d\mu'$$

where

$$A = \int_0^1 \phi(0, -\mu) d\mu$$

is the level of the scalar flux at the boundary  $x = 0$ . The

integral in this form is evaluated by using (2.10) and the

resulting equation is solved to give

$$\phi(0, -\mu) = A \frac{c}{2} \frac{H(\mu)}{(1 - \kappa\mu)} . \quad (2.28)$$

Integration of equation (2.28) with respect to  $\mu$

over the range  $(0, 1)$  provides an alternative derivation of the

normalisation integral (2.19).

With the initial values of the angular fluxes determined by equations (2.27) and (2.28) we can again attempt a solution of the transport equation (2.21) by Laplace Transform methods. The procedure is similar to that used in the preceding section and



yields for the Laplace Transform of the scalar flux the expressions

$$\bar{\phi}(\rho) = \frac{A}{(\rho - \kappa)H(-1/\rho) \left(1 - \frac{c}{2\rho} \log \left| \frac{1+\rho}{1-\rho} \right| \right)} \quad (2.29)$$

or 
$$\bar{\phi}(\rho) = \frac{A H(1/\rho)}{(\rho - \kappa)} \quad \rho \notin (-1, -\infty)$$

after using equation (2.18).

The inversion procedure for equation (2.29) is similar to that used for equation (2.22) with one important addition. The factor  $(\rho - \kappa)$  in the denominator of equation (2.29) means that there is a contribution to the scalar flux from the pole in  $\bar{\phi}(\rho)$  at  $\rho = \kappa$ . The asymptotic form of the scalar flux thus has two components and

$$\phi_{\text{asy}}(x) = B e^{\kappa x} + C e^{-\kappa x} \quad (230)$$

$$= D \sinh \kappa(x + x_0)$$

where 
$$x_0 = \frac{1}{2\kappa} \log \frac{B}{-C}.$$

From Cauchy's residue theorem

$$B = \text{residue } \{\bar{\phi}(\rho)\} \text{ at } \rho = \kappa$$

$$C = \text{residue } \{\bar{\phi}(\rho)\} \text{ at } \rho = -\kappa.$$

The residues are readily found to be

$$B = A H(1/\kappa)$$

$$C = \frac{-A}{2H(1/\kappa) \left( \frac{c}{1-\kappa^2} - 1 \right)}$$

and we have that the extrapolation length  $x_0$  is

$$x_0 = \frac{1}{2\kappa} \log \left\{ 2 [H(1/\kappa)]^2 \left[ \frac{c}{1-\kappa^2} - 1 \right] \right\} \quad (2.31)$$

whilst the ratio of the asymptotic flux to the true flux at  $x = 0$  is given by

$$\begin{aligned} \frac{\phi_{\text{asy}}(0)}{\phi(0)} &= \frac{B + C}{A} \\ &= H(1/\kappa) (1 - e^{-2\kappa x_0}). \end{aligned} \quad (2.32)$$

The absorption free case when  $c = 1$  has to be treated specially since  $\kappa$  then becomes zero. The necessary modifications to equations (2.28) through (2.32) are discussed by Auerbach (1961) though not specifically in connection with the Milne problem. For completeness we give the results for  $c = 1$  briefly. In lieu of equation (2.28) the emergent distribution becomes

$$\phi(0, -\mu) = \frac{A}{2} H(\mu) \quad (2.28a)$$

and the Laplace Transform of the scalar flux is

$$\bar{\phi}(\rho) = \frac{A}{\rho H(-1/\rho) \left( 1 - \frac{1}{2\rho} \log \left( \frac{1+\rho}{1-\rho} \right) \right)}. \quad (2.29a)$$

The singularities arise because of the double zero in the function

$$T(1/\rho) = 1 - \frac{1}{2\rho} \log \left( \frac{1+\rho}{1-\rho} \right)$$

at  $\rho = 0$ . According to the inversion formula the asymptotic

value of the scalar flux  $\phi(x)$  is

$$\phi_{\text{asy}}(x) = \text{residue} \left\{ \frac{e^{\rho x} A}{\rho H(-1/\rho) \left(1 - \frac{1}{2\rho} \log \left(\frac{1+\rho}{1-\rho}\right)\right)} \right\}_{\rho=0}.$$

Now from equation (2.12)

$$\frac{1}{H(-1/\rho)} = 1 - \frac{1}{2} \int_0^1 \frac{H(\mu)}{1-\mu\rho} d\mu$$

so near  $\rho = 0$  we expand  $(1 - \mu\rho)^{-1}$  by the binomial series and perform the integration term by term. Thus

$$\frac{1}{H(-1/\rho)} = 1 - \frac{1}{2} \sum_{n=0}^{\infty} \int_0^1 \mu^n \rho^n H(\mu) d\mu$$

$$\frac{1}{H(-1/\rho)} = - \frac{1}{2} \sum_{n=1}^{\infty} \rho^n h_n$$

since  $h_0 = 2$ .

Expanding the other terms in powers of  $\rho$  we have

$$\phi_{\text{asy}}(x) = \text{residue} \left\{ \frac{A(1+\rho x + \frac{1}{2}\rho^2 x^2 + \dots)^{\frac{1}{2}} (h_1 \rho + h_2 \rho^2 + \dots)}{\rho (\frac{1}{3}\rho^2 + \frac{1}{5}\rho^4 + \dots)} \right\}_{\rho=0}$$

$$= \text{residue} \left\{ \frac{3A}{2} \left( \frac{h_1}{\rho^2} + \frac{h_1 x + h_2}{\rho} + \dots \right) \right\}_{\rho=0}$$

$$= \frac{3A}{2} (h_1 x + h_2). \quad (2.30a)$$

The extrapolation length  $x_0$  is then given by

$$\begin{aligned} x_0 &= h_2/h_1 \\ &= .710446\dots \end{aligned} \quad (2.31a)$$

by numerical computation, whilst the ratio of the asymptotic flux to the true flux at the boundary  $x = 0$  is

$$\frac{\phi_{\text{asy}}(0)}{\phi(0)} = \frac{\frac{3A}{2} h_2}{A}$$

or 
$$\phi_{\text{asy}}(0) = (1.2305 \dots)\phi(0). \quad (2.32a)$$

Numerical calculations have been made with the formulae (2.28) - (2.32), (2.28a) - (2.32a) for values of  $c$  in the range  $0 \leq c \leq 1$  and these are in agreement with those obtained by Case, de Hoffman and Placzek (1953) using the Wiener-Hopf method.

#### 2.4 Extension to Anisotropic Scattering

We conclude this chapter by describing briefly the changes to the previous theory necessary when scattering is anisotropic in the laboratory system.

In place of (2.1) the transport equation now becomes

$$\begin{aligned} \phi(x, \mu) + \mu \frac{\partial}{\partial x} \phi(x, \mu) &= Q(x, \mu) + \frac{1}{2} \sum_{\ell=0}^{\infty} \omega_{\ell} P_{\ell}(\mu) \int_{-1}^1 P_{\ell}(\mu') \phi(x, \mu') d\mu', \\ 0 &\leq x < \infty, \\ -1 &\leq \mu \leq 1, \end{aligned} \quad (2.33)$$

where  $P_\ell(\mu)$  is the  $\ell$ -th order Legendre polynomial

$$\omega_\ell = (2\ell+1) \int_{-1}^1 P_\ell(\mu) \sigma_s(\mu) d\mu$$

$\sigma_s(\mu)$  is the cross section for scattering  
through the angle  $\cos^{-1} \mu$

and length is again measured in units for which the total  
cross section is unity.

In practice the summation over  $\ell$  is truncated after a few terms  
and if  $\omega_0 = c$ ,  $\omega_1 = \omega_2 = \omega_3 = \dots = 0$ , we recover the isotropic  
scattering equation (2.1).

The analysis proceeds in a fashion similar to that in  
section (2.1) and the reflection function  $S(\mu, \mu')$  is found to  
satisfy in place of equation (2.7) the equation

$$\begin{aligned} & \left( \frac{1}{\mu} + \frac{1}{\mu_0} \right) S(\mu, \mu_0) \\ &= \sum_{\ell} (-)^{\ell} \omega_{\ell} \left( P_{\ell}(-\mu) + \int_0^1 P_{\ell}(\mu') \frac{S(\mu, \mu')}{2\mu'} d\mu' \right) \left( P_{\ell}(-\mu_0) + \int_0^1 P_{\ell}(\mu'') \frac{S(\mu'', \mu_0)}{2\mu''} d\mu'' \right). \end{aligned} \quad (2.34)$$

Again  $S(\mu, \mu_0)$  is symmetric and equation (2.34) may be  
written

$$\left( \frac{1}{\mu} + \frac{1}{\mu_0} \right) S(\mu, \mu_0) = \sum_{\ell} (-)^{\ell} \omega_{\ell} \phi_{\ell}(\mu) \phi_{\ell}(\mu_0) \quad (2.35)$$

where  $\phi_{\ell}(\mu) = P_{\ell}(-\mu) + \int_0^1 P_{\ell}(\mu') \frac{S(\mu, \mu')}{2\mu'} d\mu'$ .

Eliminating  $S(\mu, \mu_0)$  between these equations gives

$$\begin{aligned} \phi_\ell(\mu) = & P_\ell(-\mu) + \\ & + \frac{1}{2} \sum_n (-1)^n \omega_n \mu \phi_n(\mu) \int_0^1 P_\ell(\mu') \phi_n(\mu') \frac{d\mu'}{\mu + \mu'} . \end{aligned} \quad (2.36)$$

Again we note that if  $\omega_0 = c$  is the only non-zero  $\omega_n$  then the  $\ell = 0$  equation reduces simply to the standard equation (2.10) for the isotropic scattering H-function. When the summation is truncated after  $N + 1$  terms, (2.36) is a set of  $N + 1$  integral equations for the  $\phi_0(\mu)$ ,  $\phi_1(\mu)$ , ...,  $\phi_N(\mu)$  which can be solved iteratively in the same way as solutions were obtained for equation (2.10).

Busbridge (1960) has shown that the solutions of (2.36) may be expressed

$$\phi_r(\mu) = q_r(\mu) H(\mu), \quad r = 0, 1, \dots, N$$

where each  $q_r(\mu)$  is a polynomial of degree  $N$  in  $\mu$  and  $H(\mu)$

(independent of  $r$ ) is a solution of

$$H(\mu) = 1 + \mu H(\mu) \int_0^1 \frac{\Psi_{2N}(\mu') H(\mu') d\mu'}{\mu + \mu'} ,$$

where  $\Psi_{2N}(\mu)$  is a polynomial of degree  $2N$  which depends solely on

$$\omega_0, \omega_1, \dots, \omega_N.$$

With the H-function known the scattering function  $S(\mu, \mu_0)$  can then be evaluated and the way is open to solution of the anisotropic scattering equivalent of the problems studied in section 2.3. The report by Auerbach (1961) discusses these problems for some simple anisotropic scattering models.

However the analysis is still very complex and the remark made by Davison (1957) in discussing the Wiener-Hopf method is appropriate here. The quotation from the end of Davison's section 17.4.2 reads 'If an answer of a given accuracy is required, it is usually better to use a numerical method'.

### 3. ONE GROUP THEORY FOR A FINITE SLAB

In this chapter we first discuss briefly the application of Chandrasekhar's method to finite slabs treated in one energy group. The method describes the reflection and transmission properties of the slab in terms of the X- and Y-functions developed by Chandrasekhar (1960). In deriving the equations for the functions we follow the treatment of Auerbach (1961) but they may be obtained by a variety of alternative methods, (e.g. Sobolev (1963), Mullikin (1962, 1964)), Pahor (1967), Pahor and Zweifel (1969) have shown the connection between the Chandrasekhar method and the now popular singular eigenfunction method of Case (1960).

The semi infinite medium solutions discussed in Chapter 2 are then used to develop approximations for the X- and Y-functions which will be valid for thick slabs. The study is restricted to materials with isotropic scattering, the treatment of anisotropic scattering being left until the multigroup problem is treated. We also assume that the material of the slab is non-multiplying so that  $c$ , the average number of secondary neutrons produced on a collision is restricted to  $0 \leq c \leq 1$ .

#### 3.1 X- and Y-functions for Isotropic Scattering

In the case of semi infinite slabs a scattering function  $S(\mu, \mu_0)$  was defined which was independent of  $x$  - the space co-



ordinate. In the finite slab case two functions have to be defined,  $S(x; \mu, \mu_0)$  and  $T(x; \mu, \mu_0)$  both depending on  $x$ , which correspond to the possibility of either reflecting neutrons from a slab of thickness  $x$ , or of transmitting them through the thickness  $x$ . The unit of length again has been chosen to make the total cross section unity. Thus  $(1/2\mu)S(x; \mu, \mu_0)$  with  $\mu, \mu_0 > 0$  is defined as the angular flux reflected back into the direction  $\mu$  from an incident angular flux of strength unity in the direction  $\mu_0$ . Correspondingly  $(1/2\mu)T(x; \mu, \mu_0)$  is defined for the same incident flux, as the angular flux of neutrons transmitted through the slab in direction  $\mu$  after they have made at least one collision. Since the angular flux transmitted without collision is  $\exp(-x/\mu_0)\delta(\mu-\mu_0)$  the total transmitted angular flux for this incident source is

$$e^{-x/\mu_0} \delta(\mu-\mu_0) + \frac{1}{2\mu} T(x; \mu, \mu_0).$$

Consider now as in Figure 3.1 a slab AC of thickness  $a$  with an incident angular flux on the left surface only so that

$$\phi(0, +\mu) = \delta(\mu-\mu_0) \quad 0 < \mu, \mu_0 \leq 1 \quad (3.1)$$

$$\text{and} \quad \phi(a, -\mu) = 0 \quad 0 < \mu \leq 1. \quad (3.2)$$

We imagine the slab split at B and proceed to compute angular fluxes at A, B and C.

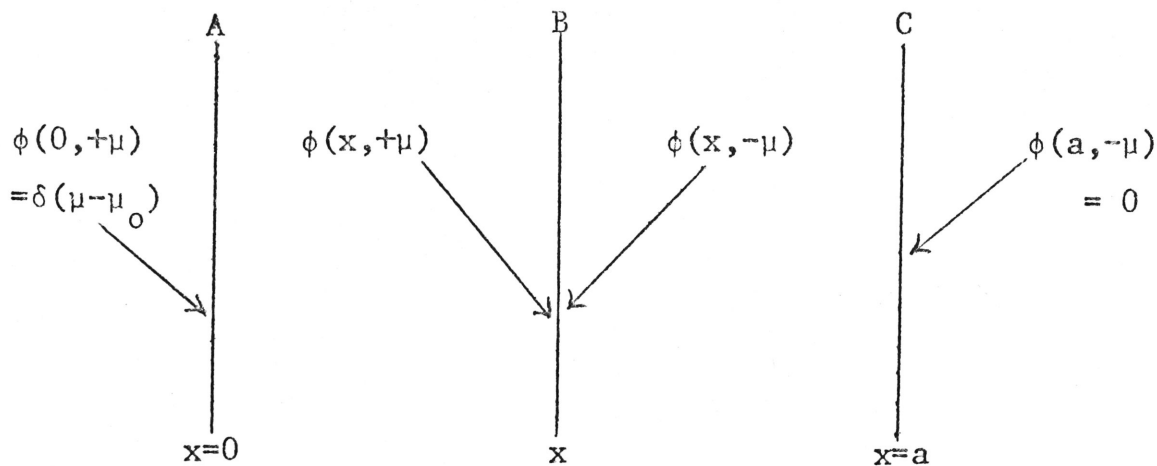


Figure 3.1

The definition of  $S$  implies that

$$\phi(x, -\mu) = \frac{1}{2\mu} \int_0^1 S(a-x; \mu, \mu') \phi(x, +\mu') d\mu' \quad (3.3)$$

(reflection from layer  $\vec{BC}$ ),

for those neutrons travelling in the sense  $\vec{BC}$  determine the angular flux  $\phi(x, +\mu)$  and these are reflected back from the layer  $BC$  of thickness  $a - x$  to give the angular flux  $\phi(x, -\mu)$ .

The definition of  $T$  implies that

$$\phi(a, +\mu) = e^{-(a-x)/\mu} \phi(x, \mu) + \frac{1}{2\mu} \int_0^1 T(a-x; \mu, \mu') \phi(x, \mu') d\mu' \quad (3.4)$$

(transmission through the layer  $\vec{BC}$ ),

and we also find that

$$\phi(x, +\mu) = e^{-x/\mu} \delta(\mu - \mu_0) + \frac{1}{2\mu} T(x; \mu, \mu_0)$$

(transmission through layer  $\vec{AB}$ );

$$+ \frac{1}{2\mu} \int_0^1 S(x; \mu, \mu') \phi(x, -\mu') d\mu' \quad (3.5)$$

(reflection from layer  $\overleftarrow{AB}$ ),

$$\phi(0, -\mu) = e^{-x/\mu} \phi(x, -\mu) + \frac{1}{2\mu} \int_0^1 T(x; \mu, \mu') \phi(x, -\mu') d\mu'$$

(transmission through layer  $\overleftarrow{AB}$ )

$$+ \frac{1}{2\mu} S(x; \mu, \mu_0) \quad (3.6)$$

(reflection from layer  $\overrightarrow{AB}$ ).

By considering the reflections from and transmissions through the whole slab  $\overrightarrow{AC}$  it follows that

$$\phi(0, -\mu) = \frac{1}{2\mu} S(a; \mu, \mu_0) \quad (3.7)$$

$$\phi(a, +\mu) = e^{-a/\mu} \delta(\mu - \mu_0) + \frac{1}{2\mu} T(a; \mu, \mu_0). \quad (3.8)$$

From these equations and the source free transport equation

$$\phi(x, \pm\mu) \pm \mu \frac{\partial \phi}{\partial x}(x, \pm\mu) = \frac{c}{2} \int_{-1}^1 \phi(x, \mu') d\mu' \quad (3.9)$$

we can determine  $S(a; \mu, \mu_0)$  and  $T(x; \mu, \mu_0)$ . The procedure is an extension of that used in section (2.1) for the semi infinite medium. Equations (3.3) through (3.6) are differentiated with respect to  $x$  and  $x$  is set equal to zero in the first pair and set

equal to  $a$  in the second pair. This gives four equations connecting the derivative of the angular fluxes at  $x = 0$  and  $x = a$ . From the transport equation (3.9) and equations (3.1) (3.2) (3.7) (3.8) these derivatives can be evaluated in terms of the functions  $S$  and  $T$ . Eliminating the derivative leads to the following four equations

$$\left(\frac{1}{\mu} + \frac{1}{\mu_0}\right) S(a; \mu, \mu_0) + \frac{\partial}{\partial a} S(a; \mu, \mu_0)$$

$$= c \left\{ 1 + \int_0^1 S(a; \mu, \mu') \frac{d\mu'}{2\mu'} \right\} \left\{ 1 + \int_0^1 S(a; \mu'', \mu_0) \frac{d\mu''}{2\mu''} \right\}$$

$$\frac{1}{\mu} T(a; \mu, \mu_0) + \frac{\partial}{\partial a} T(a; \mu, \mu_0)$$

$$= c \left\{ e^{-a/\mu_0} + \int_0^1 T(a; \mu'', \mu_0) \frac{d\mu''}{2\mu''} \right\} \left\{ 1 + \int_0^1 S(a; \mu, \mu') \frac{d\mu'}{2\mu'} \right\}$$

$$\frac{1}{\mu_0} T(a; \mu, \mu_0) + \frac{\partial}{\partial a} T(a; \mu, \mu_0)$$

$$= c \left\{ e^{-a/\mu} + \int_0^1 T(a; \mu, \mu') \frac{d\mu'}{2\mu'} \right\} \left\{ 1 + \int_0^1 S(a; \mu'', \mu_0) \frac{d\mu''}{2\mu''} \right\}$$

$$\frac{\partial}{\partial a} S(a; \mu; \mu_0)$$

$$= c \left\{ e^{-a/\mu_0} + \int_0^1 T(a; \mu'', \mu_0) \frac{d\mu''}{2\mu''} \right\} \left\{ e^{-a/\mu} + \int_0^1 T(a; \mu, \mu') \frac{d\mu'}{2\mu'} \right\} .$$

Now the reciprocity theorem of Case, de Hoffman and Placzek (1953) implies that both  $S(a;\mu,\mu_0)$  and  $T(a;\mu,\mu_0)$  are symmetric in  $\mu,\mu_0$  so when we write

$$X(a;\mu) = 1 + \int_0^1 S(a;\mu,\mu') \frac{d\mu'}{2\mu}, \quad (3.10)$$

$$Y(a;\mu) = e^{-a/\mu} + \int_0^1 T(a;\mu,\mu') \frac{d\mu'}{2\mu}, \quad (3.11)$$

the derivatives of  $S$  and  $T$  can be eliminated to give

$$\left(\frac{1}{\mu} + \frac{1}{\mu_0}\right) S(a;\mu,\mu_0) = c \left\{ X(a;\mu) X(a;\mu_0) - Y(a;\mu) Y(a;\mu_0) \right\}$$

$$\left(\frac{1}{\mu} - \frac{1}{\mu_0}\right) T(a;\mu,\mu_0) = c \left\{ X(a;\mu) Y(a;\mu_0) - X(a;\mu_0) Y(a;\mu) \right\}$$

when it follows that

$$X(a;\mu) = 1 + \frac{c\mu}{2} \int_0^1 \frac{\{X(a;\mu)X(a;\mu') - Y(a;\mu)Y(a;\mu')\}}{\mu + \mu'} d\mu', \quad (3.12)$$

$$Y(a;\mu) = e^{-a/\mu} - \frac{c\mu}{2} \int_0^1 \frac{\{X(a;\mu)Y(a;\mu') - X(a;\mu')Y(a;\mu)\}}{\mu - \mu'} d\mu'. \quad (3.13)$$

With the same incident source at  $x = 0$  the scalar fluxes at  $x = 0$  and  $x = a$  are

$$\begin{aligned} \phi(0) &= \int_0^1 \phi(0,\mu) d\mu + \int_0^1 \phi(0,-\mu) \\ &= 1 + \int_0^1 S(a;\mu,\mu_0) \frac{d\mu}{2\mu} \end{aligned}$$

and from equation (3.10)

$$\phi(0) = X(a; \mu_0). \quad (3.14)$$

In addition

$$\begin{aligned} \phi(a) &= \int_0^1 \phi(a, \mu) d\mu \\ &= e^{-a/\mu_0} + \int_0^1 T(a; \mu, \mu_0) \frac{d\mu}{2\mu} \end{aligned}$$

and from equation (3.11)

$$\phi(a) = Y(a; \mu_0). \quad (3.15)$$

These give a physical interpretation for the functions and are the definitions of the X- and Y-functions adopted by Busbridge (1960).

As  $a \rightarrow \infty$  the transmissions through a slab of thickness  $a$  tend to zero and then  $Y(a; \mu) \rightarrow 0$ , whilst  $X(a; \mu) \rightarrow H(\mu)$ , the H-function for isotropic scattering.

With the X- and Y-functions known the functions  $S(a; \mu, \mu_0)$  and  $T(a; \mu, \mu_0)$  can be evaluated and the problem of calculating reflection from or transmission through a finite slab has thus been reduced to the equivalent problem of calculating the appropriate X- or Y-functions. This problem will be our concern in the remainder of this chapter.

### 3.2 Difficulty of Numerical Solutions

At first sight it would appear that the defining equations (3.12) (3.13) can be used in an iterative procedure to evaluate the X- and Y-functions. Van de Hulst (1948) has discussed a procedure which may be used to correct each successive iterate and this correction procedure, discussed by Chandrasekhar (1948, 1949, 1960), was used with the iterative scheme in preparing the tables of Chandrasekhar, Elbert and Franklin (1952) for  $0 < c \leq 1$ ,  $0 \leq a \leq 1$ . The direct iterative scheme was discussed by Mayers (1962) who proposed a number of numerical integration schemes for avoiding the apparent ambiguity in the integrand of equation (3.13) at  $\mu' = \mu$ . Chandrasekhar (1960) and Mullikin (1964) have shown that the equations (3.12) (3.13) do not possess a unique set of solutions and Mullikin (1964) showed that the presence of extraneous solutions is the basis for numerical difficulties associated with the computation of the functions. He resolved the lack of uniqueness by showing that the solution defined by our physical interpretation (3.14) (3.15) is the solution to which the iterative schemes can converge if sufficient accuracy is taken in the numerical work, and that this solution is the only solution which is an analytic function of  $c$  in the neighbourhood of  $c = 0$ . Bellman, Kalaba and Wing (1960) pointed out that the four equations involving the derivatives of

$S(a;\mu,\mu_0)$  and  $T(a;\mu,\mu_0)$  together with the obvious initial conditions at ' $a$ ' = 0 are sufficient to compute these functions by a marching process with ' $a$ ' increasing, and the X- and Y-functions can be computed from these solutions. Computations with these differential forms of the equation have been reported by Bellman, Kalaba and Prestrud (1962).

### 3.3 Solutions for Thick Slabs

None of these standard methods is satisfactory for large values of  $a$  and for deep penetration problems very large values of  $a$  will be necessary. We shall now derive approximations to the functions  $X(a;\mu)$ ,  $Y(a;\mu)$  which will be asymptotically correct as  $a \rightarrow \infty$ .

Consider again the slab  $0 \leq x \leq a$  with boundary angular fluxes for  $0 < \mu \leq 1$

$$\phi(0,\mu) = \delta(\mu-\mu_0)$$

$$\phi(a,-\mu) = 0.$$

If solutions of the transport equation (3.9) with these boundary conditions can be found, then we have seen that

$$X(a;\mu_0) - 1 = \int_0^1 \phi(0,-\mu) d\mu \quad (3.16)$$

$$Y(a;\mu_0) = \int_0^1 \phi(a,+\mu) d\mu. \quad (3.17)$$



Calculation of the X- or Y-functions are thus seen to be special cases of the general problem of calculating weighted integrals of the angular fluxes emerging from the slab. These integrals have the general form

$$I = \int_0^1 S^*(\mu) \phi(0, -\mu) d\mu + \int_0^1 T^*(\mu) \phi(a, +\mu) d\mu \quad (3.18)$$

with

$$I = X(a; \mu_0) - 1$$

when

$$S^*(\mu) = 1$$

$$T^*(\mu) = 0$$

while

$$I = Y(a; \mu_0)$$

when

$$S^*(\mu) = 0$$

$$T^*(\mu) = 1.$$

### 3.3.1 Variational estimates for I

To estimate I we use a variational principle and evaluate the functional  $\mathcal{L}$  where

$$\begin{aligned} \mathcal{L} &= \int_0^1 S^*(\mu) \psi(0, -\mu) d\mu + \int_0^1 T^*(\mu) \psi(a, \mu) d\mu \\ &\quad - \int_0^1 \mu \psi^*(a, -\mu) \psi(a, -\mu) d\mu + \mathcal{L}_0 \end{aligned} \quad (3.19)$$

with

$$\begin{aligned}\mathcal{L}_0 &= \int_0^a dx \int_{-1}^1 \psi^*(a, \mu) \left\{ \frac{c}{2} \int_{-1}^1 \psi(x, \mu') d\mu' - \psi(x, \mu) - \mu \frac{\partial}{\partial x} \psi(x, \mu) \right\} d\mu \\ &+ \int_0^1 \mu \psi^*(0, \mu) \{ \delta(\mu - \mu_0) - \psi(0, \mu) \} d\mu.\end{aligned}\quad (3.20)$$

Now  $\mathcal{L}$  is clearly identical with I if the trial function  $\psi(x, \mu)$  satisfies the transport equation (3.9) in  $0 \leq x \leq a$  and the boundary conditions (3.1) and (3.2) for  $\phi(x, \mu)$ . However if the trial function  $\psi(x, \mu)$  differs from the correct value then the resultant change  $\delta\mathcal{L}$  in  $\mathcal{L}$  is found by direct computation to be

$$\begin{aligned}\delta\mathcal{L} &= \int_0^a dx \int_{-1}^1 \delta\psi(x, \mu) \left\{ \frac{c}{2} \int_{-1}^1 \psi^*(x, \mu') d\mu' - \psi^*(x, \mu) + \mu \frac{\partial}{\partial x} \psi^*(x, \mu) \right\} d\mu \\ &+ \int_0^1 \delta\psi(0, -\mu) \left\{ S^*(\mu) - \mu \psi^*(0, -\mu) \right\} d\mu \\ &+ \int_0^1 \delta\psi(a, \mu) \left\{ T^*(\mu) - \mu \psi^*(a, \mu) \right\} d\mu\end{aligned}$$

where  $\delta\psi(x, \mu) = \psi(x, \mu) - \phi(x, \mu)$  is the error in the trial function.

If the function  $\psi^*(x, \mu)$  is chosen to be the solution of the adjoint transport equation for  $\phi^*(x, \mu)$

$$\phi^*(x, \mu) - \mu \frac{\partial}{\partial x} \phi^*(x, \mu) = \frac{c}{2} \int_{-1}^1 \phi^*(x, \mu') d\mu' \quad 0 \leq x \leq a$$

with boundary conditions

$$\phi^*(0, -\mu) = \frac{1}{\mu} S^*(\mu)$$

$$\phi^*(a, +\mu) = \frac{1}{\mu} T^*(\mu)$$

then clearly  $\delta\mathcal{L}$  is zero. In the same way  $\mathcal{L}$  has zero variation about the correct value for errors in  $\psi^*(x, \mu)$  provided that  $\psi(x, \mu)$  is chosen to be the correct solution  $\phi(x, \mu)$ . In the sense of Lewins (1965a) (1965b), the functional  $\mathcal{L}$  thus supplies a suitable estimator for I. The customary procedure for use of the variational expression (3.19) is to choose for  $\psi(x, \mu)$  and  $\psi^*(x, \mu)$  parameter dependent trial functions and then to select the parameters in such a way as to make  $\mathcal{L}$  stationary with respect to variation of these parameters. However we are interested here in obtaining semi-analytic forms for the X- and Y-functions and the customary method is not satisfactory.

An alternative course will therefore be followed by simply selecting for the trial functions expressions which are reasonable approximations to the true neutron angular flux and adjoint function, substituting these into equation (3.19) and accepting the results as approximations to the integral (3.18).

We are seeking approximations which will be valid for slabs of large thickness  $a$  and, for such systems, numerical studies show that the angular flux  $\phi(x, \mu)$  for the finite slab is well approximated (except near  $x = a$ ) by the angular flux appropriate

to the semi infinite system  $0 \leq x < \infty$ . Physically the flux near the source plane  $x = 0$  is not strongly affected by the presence or absence of material beyond  $x = a \gg 0$ . Since a corresponding result will be true for solutions of the adjoint equation an appropriate set of trial functions will be the flux and adjoint functions for correctly chosen semi infinite medium problems.

When estimating either  $X(a; \mu_0)$  or  $Y(a; \mu_0)$  by means of equations (3.16) (3.19) we shall therefore choose as a trial function  $\psi(x, \mu)$  the solution to the semi infinite medium albedo problem discussed in section 2.3.2. That is,  $\psi(x, \mu)$  satisfies the source free transport equation in  $0 \leq x < \infty$  and therefore throughout the range  $0 \leq x \leq a$ . In addition

$$\begin{aligned} \psi(0, \mu) &= \delta(\mu - \mu_0) \quad \mu > 0, \\ \psi(0, -\mu) &= \frac{c}{2} \mu_0 \frac{H(\mu)H(\mu_0)}{\mu + \mu_0}. \end{aligned}$$

With this trial function the term  $\mathcal{L}_0$  defined in equation (3.20) is identically zero and the trial functions then need only be evaluated at the boundaries  $x = 0$  and  $x = a$ . We make one further assumption, namely that  $a$  is large enough for the trial function  $\psi(a, \mu)$  to be adequately approximated by the asymptotic solution described by equations (2.24) and (2.25), so that we assume

$$\psi(a, \mu) = \frac{c}{2} \frac{e^{-\kappa a}}{(1 - \kappa \mu)} \alpha(\mu_0) \quad (3.21)$$

where

$$\alpha(\mu_0) = \frac{\mu_0 H(\mu_0) (1 - \kappa^2) \kappa}{(1 - \kappa \mu_0) (\kappa^2 + c - 1) H(\frac{1}{\kappa})} \quad (3.22)$$

and  $\kappa$  is the inverse relaxation length.

### 3.3.2 Solutions for adjoint semi infinite albedo problem

At this point it is appropriate to develop quickly the solution to the adjoint semi infinite medium albedo problem defined by the adjoint equation

$$\phi^*(x, \pm\mu) \mp \mu \frac{\partial}{\partial x} \phi^*(x, \pm\mu) = \frac{c}{2} \int_{-1}^1 \phi^*(x, \mu') d\mu' \quad (3.23)$$

with additional conditions

$$\phi^*(0, -\mu) = \delta(\mu - \mu_1) \quad 0 < \mu, \mu_1 \leq 1 \quad (3.24)$$

$$\lim_{x \rightarrow \infty} \phi^*(x, \mu) = 0.$$

Comparison of these equations with the regular transport equation (2.21) and the boundary condition for the regular albedo problem discussed in section 2.3.2 lets us write down immediately that

$$\begin{aligned} \phi^*(0, +\mu) &= \frac{1}{2\mu} S(\mu, \mu_1) \\ &= \frac{c}{2} \frac{\mu_1}{\mu + \mu_1} H(\mu) H(\mu_1) \end{aligned} \quad (3.25)$$

from equations (2.5) (2.9), whilst for large  $x$ , the asymptotic solution by comparison with equation (3.21) is simply

$$\phi_{\text{asy}}^*(x, \mu) = \frac{c}{2} \frac{e^{-\kappa x}}{1 + \kappa \mu} \alpha(\mu_1). \quad (3.26)$$

### 3.3.3 Approximation of $X(a; \mu_0)$

From equations (3.16) and (3.18) it is clear that the adjoint function for calculation of  $X(a; \mu_0)$  should satisfy the adjoint transport equation (3.23) with boundary conditions

$$\left. \begin{aligned} \phi^*(0, -\mu) &= \frac{1}{\mu} S^*(\mu) = \frac{1}{\mu} \\ \phi^*(a, +\mu) &= \frac{1}{\mu} T^*(\mu) = 0 \end{aligned} \right\}. \quad (3.27)$$

The approximation we choose for  $\phi^*(x, \mu)$  is the solution for the semi infinite medium  $0 \leq x < \infty$  which satisfies the boundary condition (3.27), and we again assume that  $a$  is large enough that the adjoint function has settled down into an asymptotic distribution at  $x = a$ . This approximate solution we generate by integration of the solution for the semi infinite medium albedo problem studied in section 3.3.2. Denoting for the moment this latter function by  $f(\mu_1; x, \mu)$  we have that

$$f(\mu_1; 0, -\mu) = \delta(\mu - \mu_1) \quad 0 < \mu, \mu_1 \leq 1$$

$$f(\mu_1; 0, +\mu) = \frac{c}{2} \frac{\mu_1}{\mu + \mu_1} H(\mu) H(\mu_1).$$

Since our trial function is to satisfy (3.27) we see that

the appropriate choice is

$$\psi^*(x, \mu) = \int_0^1 f(\mu_1; x, \mu) \frac{d\mu_1}{\mu_1}$$

so that

$$\begin{aligned} \psi^*(0, -\mu) &= \int_0^1 \delta(\mu - \mu_1) \frac{d\mu_1}{\mu_1} \\ &= \frac{1}{\mu} \end{aligned} \quad (3.28)$$

We have then for this trial function

$$\begin{aligned} \psi^*(0, \mu) &= \int_0^1 \frac{d\mu_1}{\mu_1} \frac{c}{2} \frac{\mu_1}{\mu + \mu_1} H(\mu) H(\mu_1) \\ &= \frac{H(\mu) - 1}{\mu} \end{aligned} \quad (3.29)$$

from equation (2.12), and

$$\psi^*(a, \mu) = \int_0^1 \frac{d\mu_1}{\mu_1} \frac{ce^{-\kappa a}}{2(1+\kappa\mu)} \alpha(\mu_1)$$

for large  $a$ .

Now

$$\begin{aligned} \int_0^1 \frac{\alpha(\mu_1)}{\mu_1} d\mu_1 &= \int_0^1 \frac{\mu_1^{H(\mu_1)} (1-\kappa^2)\kappa}{\mu_1 (1-\kappa\mu_1) (\kappa^2+c-1) H(\frac{1}{\kappa})} d\mu_1 \\ &= \frac{(1-\kappa^2)\kappa}{(\kappa^2+c-1) H(\frac{1}{\kappa})} \int_0^1 \frac{\mu_1^{H(\mu_1)-1}}{(1-\kappa\mu_1)} d\mu_1 \\ &= \frac{(1-\kappa^2)\kappa}{(\kappa^2+c-1) H(\frac{1}{\kappa})} \cdot \frac{2}{c} \end{aligned}$$

from equation (2.19). We have finally, for large  $a$  that

$$\psi^*(a, \mu) = \frac{(1-\kappa^2)\kappa e^{-\kappa a}}{(\kappa^2+c-1)H(\frac{1}{\kappa})(1+\kappa\mu)} \quad (3.30)$$

We now substitute these expressions into equation (3.19) and get

$$\begin{aligned} X(a; \mu_0) - 1 &\approx \mathcal{L} \\ &= \int_0^1 \frac{c}{2} \cdot \frac{\mu_0 H(\mu_0) H(\mu)}{\mu + \mu_0} d\mu \\ &\quad - \int_0^1 \frac{(1-\kappa^2)\kappa e^{-\kappa a}}{(\kappa^2+c-1)H(\frac{1}{\kappa})(1-\kappa\mu)} \cdot \frac{c\mu_0 H(\mu_0)(1-\kappa^2)\kappa e^{-\kappa a}}{2(1-\kappa\mu_0)(\kappa^2+c-1)H(\frac{1}{\kappa})(1+\kappa\mu)} d\mu \end{aligned}$$

The first integral is evaluated with the help of equation (2.10) and we then have

$$\begin{aligned} X(a; \mu_0) - 1 &\approx H(\mu_0) - 1 \\ &\quad - \frac{c}{2} \left\{ \frac{\kappa(1-\kappa^2)e^{-\kappa a}}{(\kappa^2+c-1)H(\frac{1}{\kappa})} \right\}^2 \frac{\mu_0 H(\mu_0)}{1-\kappa\mu_0} \int_0^1 \frac{\mu d\mu}{(1-\kappa^2\mu^2)} \end{aligned}$$

This last integral is elementary and the approximation reduces to

$$X(a; \mu_0) \approx H(\mu_0) \left\{ 1 + \frac{c}{4} \frac{\log(1-\kappa^2)}{(1-\kappa\mu_0)} \left( \frac{(1-\kappa^2)e^{-\kappa a}}{(\kappa^2+c-1)H(\frac{1}{\kappa})} \right)^2 \right\} \quad (3.31)$$

a result first obtained by the candidate by a slightly different procedure (Clancy, 1969).



### 3.3.4 Approximation for $Y(a; \mu_0)$

Again from equations (3.12) and (3.18) we see that the adjoint function for calculation of  $Y(a; \mu_0)$  should satisfy the adjoint transport equation (3.23) with boundary conditions

$$\left. \begin{aligned} \phi^*(a, +\mu) &= \frac{1}{\mu} T^*(\mu) = \frac{1}{\mu} \\ \phi^*(0, -\mu) &= \frac{1}{\mu} S^*(\mu) = 0 \end{aligned} \right\} \quad (3.32)$$

but we choose as an approximation to this, a function which satisfies the boundary condition (3.32) and is a solution to the adjoint transport equation in the semi infinite medium  $-\infty < x \leq a$ . This adjoint function is similar to that used in the previous problem but reflected completely about the plane  $x = \frac{a}{2}$ .

The function  $\psi^*(a, -\mu)$  needed for this calculation is thus identical with the  $\phi^*(0, +\mu)$  of the previous section and from equation (3.29) we see that for this problem

$$\psi^*(a, -\mu) = \frac{H(\mu) - 1}{\mu} .$$

Substituting these expressions into equation (3.19) gives

$$\begin{aligned} Y(a; \mu_0) &\approx \mathcal{L} \\ &= \int_0^1 \frac{c e^{-\kappa a}}{2(1-\kappa\mu)} \alpha(\mu_0) d\mu \\ &\quad - \int_0^1 [H(\mu) - 1] \frac{c e^{-\kappa a}}{2(1+\kappa\mu)} \alpha(\mu_0) d\mu \\ &= \frac{c}{2} e^{-\kappa a} \alpha(\mu_0) \left\{ \int_0^1 \frac{d\mu}{1-\kappa\mu} + \int_0^1 \frac{d\mu}{1+\kappa\mu} - \int_0^1 \frac{H(\mu)}{1+\kappa\mu} d\mu \right\} . \end{aligned}$$

The first two of these integrals are elementary and combine together to give  $\frac{1}{\kappa} \log \left( \frac{1+\kappa}{1-\kappa} \right)$  which from the equation defining  $\kappa$  is simply  $\frac{2}{c}$ . So

$$\begin{aligned} Y(a; \mu_0) &\approx e^{-\kappa a} \alpha(\mu_0) \left\{ 1 - \frac{c}{2\kappa} \int_0^1 \frac{H(\mu)}{\mu + \frac{1}{\kappa}} d\mu \right\} \\ &= e^{-\kappa a} \alpha(\mu_0) \frac{1}{H(\frac{1}{\kappa})} \end{aligned} \quad (3.33)$$

from equation (2.12). The final approximation is then

$$Y(a; \mu_0) \approx \frac{\kappa \mu_0 H(\mu_0) (1-\kappa^2) e^{-\kappa a}}{(1-\kappa \mu_0) (\kappa^2 + c - 1) [H(\frac{1}{\kappa})]^2} \quad (3.34)$$

again in agreement with Clancy (1969).

It is interesting to note that this approximation can be obtained by an independent argument which does not have recourse to the variational principle. It is again assumed that the slab is thick enough that the scalar flux near the centre of the slab can be adequately described by the asymptotic solution found in section 2.3.2. From equation (2.24) it follows that this is

$$\phi(x) = \alpha(\mu_0) e^{-\kappa x}.$$

Again if the slab is thick enough this expression will adequately approximate the scalar flux for the Milne problem in the semi infinite medium  $-\infty < x \leq a$ .

From equation (2.30) we see that the asymptotic form for the scalar flux in this problem will be

$$\phi(x) = B e^{\kappa(a-x)}$$

where  $B = H(\frac{1}{\kappa})\phi(a)$  and where  $\phi(a)$  is the scalar flux at the boundary  $x = a$ . For the finite slab with boundary flux  $\phi(0, \mu) = \delta(\mu - \mu_0)$  we have seen that  $\phi(a)$  is identical with  $Y(a; \mu_0)$  so that the second asymptotic form of the scalar flux is

$$\phi(x) = H(\frac{1}{\kappa})Y(a; \mu_0)e^{\kappa(a-x)}.$$

Since the two expressions for the asymptotic flux must be equal it follows that

$$\alpha(\mu_0)e^{-\kappa x} = H(\frac{1}{\kappa})Y(a; \mu_0)e^{\kappa(a-x)}$$

or

$$Y(a; \mu_0) = \alpha(\mu_0)e^{-\kappa a} \frac{1}{H(\frac{1}{\kappa})}$$

which is simply equation (3.33) again.

### 3.3.5 The conservative case

If there is no absorption and  $c$  becomes unity, the approximations in equations (3.31) and (3.34) become indeterminate, since  $\kappa$  becomes zero. Two procedures can then be followed. We can use as trial functions the semi-infinite medium solutions appropriate to the absorption free medium or alternatively take the limits of equations (3.31) and (3.34) as  $\kappa$  tends to zero.

Either procedure leads to the expressions

$$X(a; \mu_0) = (1 - \frac{3}{4} \mu_0) H(\mu_0)$$

$$Y(a; \mu_0) = 0$$

but these are clearly unsatisfactory as they are independent of the thickness  $a$ . This poor result is not however surprising since the alternative procedure described at the end of section 3.3.4 cannot be followed for the conservative case. When  $c = 0$  the asymptotic distribution set up far from the source plane  $x = 0$  will be

$$\phi(x) = \sqrt{3} \mu_0 H(\mu_0) \quad x \gg 0$$

which is independent of position. On the other hand the asymptotic distribution for the Milne problem in  $-\infty < x \leq a$  has the form

$$\phi(x) = \frac{\sqrt{3}}{2} \phi(a) \{a - x + 0.7104 \dots\} \quad x \ll a$$

and there is no way to match the two asymptotic forms.

### 3.3.6 Comparison with tabulated values

To test the accuracy of the approximations embodied in equations (3.31) and (3.34) their values have been compared with those tabulated by Mayers (1962) for

$c = 0.80$	$0.90$	$0.95$
$a = 2.5$	$2.0, 5.0$	$2.0, 4.0, 10.0.$

The results are displayed in Table 3.1 which also gives the

percentage error in the approximations. Provided  $a > 5.0$  the agreement is satisfactory and the approximations may be used with some confidence. For  $a < 5.0$  the approximations would be of value as initial guesses in an iterative scheme for calculating  $X(a;\mu)$  and  $Y(a;\mu)$ .

TABLE 3.1

COMPARISON OF  $X(a;\mu)$  AND  $Y(a;\mu)$  VALUES FROM EQUATIONS 3.31  
AND 3.34 WITH ACCURATE VALUES FROM MAYERS (1962)

$\mu$	$X(a;\mu)$			$Y(a;\mu)$		
	Exact	Eqn(3.31)	Error(%)	Exact	Eqn(3.34)	Error(%)
$c = 0.80, a = 2.5$						
0.0	1.0	1.0	-	0.0	0.0	-
0.1	1.1384	1.1384	0.0	0.0088	0.0083	-6.0
0.2	1.2276	1.2276	0.0	0.0208	0.0195	-6.5
0.3	1.2988	1.2988	0.0	0.0365	0.0337	-8.3
0.4	1.3583	1.3583	0.0	0.0578	0.0517	-10.6
0.5	1.4092	1.4092	0.0	0.0861	0.0745	-13.4
0.6	1.4532	1.4533	0.0	0.1213	0.1038	-14.4
0.7	1.4917	1.4918	0.0	0.1622	0.1420	-12.5
0.8	1.5256	1.5253	0.0	0.2071	0.1936	-6.5
0.9	1.5556	1.5540	-0.1	0.2544	0.2663	+4.7
1.0	1.5824	1.5778	-0.3	0.3030	0.3754	+23.9
$c = 0.90, a = 2.0$						
0.0	1.0	1.0	-	0.0		-
0.1	1.1689	1.1682	-0.1	0.0211	0.0198	-6.2
0.2	1.2839	1.2822	-0.1	0.0496	0.0463	-6.7
0.3	1.3783	1.3756	-0.2	0.0868	0.0794	-8.5
0.4	1.4585	1.4546	-0.3	0.1352	0.1200	-11.2
0.5	1.5274	1.5224	-0.3	0.1941	0.1691	-12.9
0.6	1.5872	1.5805	-0.4	0.2606	0.2283	-12.4
0.7	1.6392	1.6297	-0.6	0.3312	0.2998	-9.5
0.8	1.6848	1.6705	-0.8	0.4031	0.3865	-4.1
0.9	1.7249	1.7028	-1.3	0.4743	0.4927	+3.9
1.0	1.7605	1.7459	-0.8	0.5437	0.6248	+14.9
$c = 0.90, a = 5.0$						
0.0	1.0	1.0	0.0	0.0	0.0	0.0
0.1	1.1720	1.1720	0.0	0.0041	0.0041	-0.0
0.2	1.2911	1.2912	+0.0	0.0096	0.0096	-0.0
0.3	1.3908	1.3907	-0.0	0.0165	0.0164	-0.6
0.4	1.4776	1.4775	-0.0	0.0250	0.0248	-0.8
0.5	1.5548	1.5546	-0.0	0.0352	0.0350	-0.6
0.6	1.6242	1.6239	-0.0	0.0477	0.0472	-1.0
0.7	1.6871	1.6868	-0.0	0.0628	0.0620	-1.3
0.8	1.7446	1.7441	-0.0	0.0807	0.0799	-1.0
0.9	1.7973	1.7966	-0.0	0.1016	0.1019	+0.3
1.0	1.8458	1.8448	-0.1	0.1254	0.1292	+3.0

TABLE 3.1 (Continued)

$\mu$	$X(a;\mu)$			$Y(a;\mu)$		
	Exact	Eqn (3.31)	Error(%)	Exact	Eqn (3.34)	Error(%)
$c = 0.95, a = 2.0$						
0.0	1.0	1.0	-	0.0	0.0	-
0.1	1.1879	1.849	-0.3	0.0276	0.0250	-9.4
0.2	1.3203	1.3132	-0.5	0.0647	0.0583	-9.7
0.3	1.4312	1.4191	-0.8	0.1121	0.0996	-11.2
0.4	1.5268	1.5091	-1.2	0.1718	0.1492	-13.2
0.5	1.6098	1.5856	-1.5	0.2423	0.2078	-14.2
0.6	1.6822	1.6502	-1.9	0.3201	0.2761	-13.7
0.7	1.7457	1.7035	-2.4	0.4016	0.3554	-11.5
0.8	1.8015	1.7459	-3.1	0.4838	0.4469	-7.6
0.9	1.8508	1.7774	-4.0	0.5646	0.5524	-2.2
1.0	1.8946	1.7974	-5.1	0.6428	0.6742	+4.9
$c = 0.95, a = 4.0$						
0.0	1.0	1.0	-	0.0	0.0	-
0.1	1.1937	1.1930	-0.1	0.0118	0.0117	-0.8
0.2	1.3320	1.3320	-0.1	0.0276	0.0273	-1.1
0.3	1.4545	1.4514	-0.2	0.0472	0.0466	-1.3
0.4	1.5621	1.5574	-0.3	0.0708	0.0699	-1.3
0.5	1.6594	1.6529	-0.4	0.0989	0.0973	-1.6
0.6	1.7481	1.7396	-0.5	0.1318	0.1293	-1.9
0.7	1.8296	1.8186	-0.6	0.1697	0.1664	-1.9
0.8	1.9046	1.8907	-0.7	0.2123	0.2092	-1.5
0.9	1.9737	1.9563	-0.9	0.2589	0.2586	-0.1
1.0	2.0376	2.0158	-1.1	0.3090	0.3156	+2.1
$c = 0.95, a = 10.0$						
0.0	1.0	1.0	-	0.0	0.0	-
0.1	1.1952	1.1952	0.0	0.0013	0.0012	-0.0
0.2	1.3373	1.3373	0.0	0.0028	0.0028	0.0
0.3	1.4603	1.4604	+0.0	0.0047	0.0048	+2.0
0.4	1.5708	1.5708	0.0	0.0071	0.0072	+1.4
0.5	1.6716	1.6716	0.0	0.0099	0.0100	+1.1
0.6	1.7644	1.7644	0.0	0.0132	0.0133	+0.8
0.7	1.8506	1.8506	0.0	0.0169	0.0171	+1.2
0.8	1.9309	1.9309	0.0	0.0213	0.0215	+0.9
0.9	2.0061	2.0060	-0.0	0.0263	0.0265	+0.8
1.0	2.0766	2.0765	-0.0	0.0321	0.0323	+0.6

#### 4. MULTIGROUP THEORY FOR A SEMI INFINITE MEDIUM

Whilst the solution of neutron transport problems in one energy group can be a mathematically pleasing exercise the solutions are of limited value when discussing realistic problems. We therefore turn in this chapter to the more general problem of energy dependent transport theory and go immediately to a multi-group representation.

It is only in recent years that exact solution to any but trivial multigroup transport problems have been obtained. The first successful method was the singular eigenfunction approach of Case and Zweifel (1967) which was used to solve the infinite medium Green's function problem for two groups (Siewert and Shieh, 1967) and N-groups (Yoshimura and Katsuragi, 1968). Until 1969 the solution of half space problems was restricted to very special cases, in either two groups (Zelazny and Kuszell, 1961) or for N-group problems with severe restrictions on the elements of the energy transfer matrix (Siewert and Zweifel, 1966; Leonard and Ferziger, 1966). Pahor (1968) found the emerging distributions for the energy dependent albedo and Milne problems (for thermal neutrons with an isotropic degenerate scattering kernel) using a generalisation of the Chandrasekhar method, and Shultis (1969) generalised this work to handle anisotropic scattering while still retaining a restriction to scattering kernels which obey



a detailed balance condition. Finally Pahor and Shultis (1969) developed a theory (restricted to isotropic scattering) to solve half space problems for a general transfer matrix using again a combination of Case's singular eigenfunctions and a generalised Chandrasekhar method.

In this chapter we proceed to develop a theory for the semi infinite medium with arbitrarily anisotropic scattering and (at least initially) restrict the transfer matrix only by the requirement that the material be non-multiplying. (This corresponds to the restriction in the one group case that  $C$ , the average number of secondary neutrons produced per collision, should not be greater than unity). At a later stage the transfer matrix will be further restricted so as to disallow neutron transfers from any group to groups of higher energy. A preliminary account of this work is given by Clancy (1970).

#### 4.1 Generalisation of Chandrasekhar's Method

The analysis to follow is simplified by use of matrix and vector notation, so that for  $N$ -group problems the  $N$  separate group angular fluxes are collected into a column vector  $\underline{\phi}(x, \mu)$  whose elements are  $\phi_i(x, \mu)$   $i = 1, 2, \dots, N$ . Further, a set of transfer matrices  $\underline{C}^{\ell}$  are defined, so that  $[\underline{C}^{\ell}]_{ij}$ , the  $i, j$  component of  $\underline{C}^{\ell}$  is  $(2\ell+1)\sigma_{ij}^{\ell}$ , where  $\sigma_{ij}^{\ell}$  is the  $\ell$ -th term of the Legendre polynomial expansion of the differential scattering cross section from group

j to group i, suitably modified if the material is fissionable to allow for fission transfers into group i. Finally the diagonal matrix  $\Sigma$  is defined to have components  $\delta_{ij} \sigma_i$  where  $\sigma_i$  is the total cross section in group i and  $\delta_{ij}$  is the Kronecker delta. With this notation the N-group plane geometry transport equation for the semi infinite region  $0 \leq x < \infty$  can be written in the absence of free sources as

$$\Sigma \phi(x, \mu) + \mu \frac{\partial}{\partial x} \phi(x, \mu) = \frac{1}{2} \sum_{\ell=0}^{\infty} P_{\ell}(\mu) C_{\ell}^{\ell} \int_{-1}^1 P_{\ell}(\mu') \phi(x, \mu') d\mu'. \quad (4.1)$$

We are concerned with a homogeneous medium so that only the angular fluxes in equation (4.1) depend on x, and in practice the summation over  $\ell$  is truncated after a few terms and ranges from  $\ell = 0$  to  $\ell = L$  in a  $P_L$  scattering approximation.

The invariance principle states that the reflected flux from a homogeneous half space is unchanged by the addition (or subtraction) of layers of arbitrary thickness to (or from) the medium. Thus separating the angular fluxes into forward moving components  $\phi(x, +\mu)$  and backward moving components  $\phi(x, -\mu)$  these are related in the absence of internal sources by the equation

$$\phi(x, -\mu) = \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \phi(x, +\mu') d\mu' \quad 0 < \mu \leq 1 \quad (4.2)$$

by analogy with equation (2.2). If fixed sources are present in

the half space it will be necessary to add to equation (4.2) the term  $\phi_x(x, -\mu)$  to account for neutrons making their first passage across the x-plane in the backward direction. The reflection matrix  $S(\mu, \mu')$  is independent of x and of any sources and can be evaluated by considering the solution of equation (4.1) with the imposed boundary conditions

$$\lim_{x \rightarrow \infty} \phi(x, \mu) = 0 \quad (4.3)$$

$$\phi(0, \mu) = E^m \delta(\mu - \mu_0) \quad 0 < \mu, \mu_0 \leq 1 \quad (4.4)$$

where the components of  $E^m$  are  $\delta_{1m}, \delta_{2m}, \delta_{3m}, \dots, \delta_{Nm}$ . These boundary conditions represent the physical situation of a monodirectional beam of neutrons in group m incident onto the half space with direction cosine  $\mu_0$ . The emerging angular fluxes in any group are then given in terms of the elements  $S_{ij}(\mu, \mu')$  of the reflection matrix by

$$\phi(0, -\mu) = \frac{1}{2\mu} S(\mu, \mu_0) E^m$$

or

$$\phi_i(0, -\mu) = \frac{1}{2\mu} S_{im}(\mu, \mu_0) \quad i = 1, 2, \dots, N. \quad (4.5)$$

#### 4.2 Determination of $S(\mu, \mu_0)$

To obtain an equation for  $S$  we first differentiate equation (4.2) with respect to x and set  $x = 0$ , giving

$$\phi(0, -\mu) = \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \phi(0, +\mu') d\mu' \quad (4.6)$$

the dot ' denoting derivative with respect to  $x$ . Equation

(4.1) may, at  $x = 0$ , be written in the form

$$\begin{aligned} \dot{\phi}(0, \mu) = & -\frac{1}{\mu} \Sigma \phi(0, \mu) + \frac{1}{2\mu} \sum_{\ell} P_{\ell}(\mu) C_{\ell}^{\ell} \int_0^1 P_{\ell}(\mu') \phi(x, \mu') d\mu' \\ & + \frac{1}{2\mu} \sum_{\ell} P_{\ell}(\mu) C_{\ell}^{\ell} \int_0^1 P_{\ell}(-\mu') \phi(x, -\mu') d\mu' \end{aligned}$$

and then substitution of equations (4.4, 4.5) gives the following expressions for the derivatives at  $x = 0$ :-

$$\begin{aligned} \dot{\phi}(0, \mu) = & -\frac{1}{\mu} \delta(\mu - \mu_0) \Sigma E^m + \frac{1}{2\mu} \sum_{\ell} P_{\ell}(\mu) C_{\ell}^{\ell} E^m P_{\ell}(\mu_0) \\ & + \frac{1}{2\mu} \sum_{\ell} P_{\ell}(\mu) C_{\ell}^{\ell} \int_0^1 P_{\ell}(-\mu') S(\mu, \mu_0) \frac{d\mu'}{2\mu} E^m \\ \dot{\phi}(0, -\mu) = & \frac{1}{2\mu^2} \Sigma S(\mu, \mu_0) E^m - \frac{1}{2\mu} \sum_{\ell} P_{\ell}(-\mu) C_{\ell}^{\ell} E^m P_{\ell}(\mu_0) \\ & - \frac{1}{2\mu} \sum_{\ell} P_{\ell}(-\mu) C_{\ell}^{\ell} \int_0^1 P_{\ell}(-\mu') S(\mu, \mu_0) \frac{d\mu'}{2\mu} E^m. \end{aligned}$$

If these forms are inserted into equation (4.6) it follows after some tedious manipulations that

$$\begin{aligned} & \left( \frac{1}{\mu} \Sigma S(\mu, \mu_0) + \frac{1}{\mu_0} S(\mu, \mu_0) \Sigma \right) E^m \\ = & \sum_{\ell} \left\{ P_{\ell}(-\mu) + \int_0^1 P_{\ell}(\mu') S(\mu, \mu') \frac{d\mu'}{2\mu} \right\} C_{\ell}^{\ell} \left\{ P_{\ell}(\mu_0) + \int_0^1 P_{\ell}(-\mu'') S(\mu'', \mu_0) \frac{d\mu''}{2\mu''} \right\} E^m. \end{aligned}$$

Since the last equation is true for each  $m = 1, 2, \dots, N$  the vector  $\tilde{E}^m$  may be cancelled out from both sides to give the equation

$$\frac{1}{\mu} \tilde{\Sigma} S(\mu, \mu_o) + \frac{1}{\mu_o} S(\mu, \mu_o) \tilde{\Sigma} = \sum_{\ell} (-)^{\ell} \tilde{U}^{\ell}(\mu) \tilde{C}^{\ell} \tilde{V}^{\ell}(\mu_o) \quad (4.7)$$

where

$$\tilde{U}^{\ell}(\mu) = P_{\ell}(-\mu) \tilde{I} + \int_0^1 P_{\ell}(+\mu') \tilde{S}(\mu, \mu') \frac{d\mu'}{2\mu'} \quad (4.8)$$

$$\tilde{V}^{\ell}(\mu) = P_{\ell}(-\mu) \tilde{I} + \int_0^1 P_{\ell}(+\mu') \tilde{S}(\mu', \mu) \frac{d\mu'}{2\mu'} \quad (4.9)$$

and  $\tilde{I}$  is the  $N \times N$  unit matrix.

Writing equation (4.7) element by element we have

$$\left( \frac{\sigma_m}{\mu} + \frac{\sigma_n}{\mu_o} \right) S_{mn}(\mu, \mu_o) = \sum_{\ell} (-)^{\ell} \sum_{ij} \tilde{U}_{mi}^{\ell}(\mu) \tilde{C}_{ij}^{\ell} \tilde{V}_{jn}^{\ell}(\mu_o) \quad (4.7a)$$

so that the elements of the matrix  $S(\mu, \mu_o)$  can be evaluated from the elements of  $\tilde{U}^{\ell}(\mu)$  and  $\tilde{V}^{\ell}(\mu)$ .

From equations (4.3) and (4.5) the various Legendre moments of the angular flux at  $x = 0$  can be computed immediately so that

$$\begin{aligned} \int_0^1 P_{\ell}(\mu) \tilde{\phi}(0, \mu) d\mu &= \int_0^1 P_{\ell}(\mu) \tilde{\phi}(0, \mu) d\mu + \int_0^1 P_{\ell}(-\mu) \tilde{\phi}(0, -\mu) d\mu \\ &= \left[ P_{\ell}(\mu_o) \tilde{I} + \int_0^1 P_{\ell}(-\mu) \tilde{S}(\mu, \mu_o) \frac{d\mu}{2\mu} \right] \tilde{E}^m \\ &= (-)^{\ell} \tilde{V}^{\ell}(\mu_o) \tilde{E}^m \end{aligned} \quad (4.10)$$

and, in particular, the scalar flux at  $x = 0$  is

$$\phi(0) = \tilde{V}^0(\mu_0) \tilde{E}^m. \quad (4.10a)$$

Equation (4.10) gives a physical interpretation for the matrices  $\tilde{V}^k(\mu)$ .

Using an outer product notation where the matrix equation

$$\tilde{D} = \tilde{A} * \tilde{B}$$

is to be interpreted as

$$D_{ij} = A_{ij} \cdot B_{ij} \quad i, j = 1, 2, \dots, N.$$

$\tilde{S}$  may be eliminated between equations (4.7), (4.8), (4.9) to give for  $k = 0, 1, 2, \dots$

$$\begin{aligned} \tilde{U}^k(\mu) &= P_k(-\mu) \tilde{I} \\ &+ \frac{\mu}{2} \sum_{\ell} (-)^{\ell} \int_0^1 P_k(\mu') \tilde{A}(\mu, \mu') * (\tilde{U}^{\ell}(\mu) \tilde{C}^{\ell} \tilde{V}^{\ell}(\mu')) d\mu' \end{aligned} \quad (4.11)$$

$k = 0, 1, \dots, N$

$$\begin{aligned} \tilde{V}^k(\mu) &= P_k(-\mu) \tilde{I} \\ &+ \frac{\mu}{2} \sum_{\ell} (-)^{\ell} \int_0^1 P_k(\mu') \tilde{A}(\mu, \mu') * (\tilde{U}^{\ell}(\mu') \tilde{C}^{\ell} \tilde{V}^{\ell}(\mu)) d\mu' \end{aligned} \quad (4.12)$$

$k = 0, 1, 2, \dots, N$

where the elements of the matrix  $A(\mu, \mu')$  are

$$A_{ij}(\mu, \mu') = \frac{1}{\mu\sigma_j + \mu'\sigma_i}.$$

Written out in full, equations (4.11), (4.12) become

$$U_{mn}^k(\mu) = P_k(-\mu)\delta_{mn} + \frac{\mu}{2} \sum_{\ell} (-)^{\ell} \sum_{i,j=1}^N U_{mi}^{\ell}(\mu) C_{ij}^{\ell} \int_0^1 P_k(\mu') V_{jn}^{\ell}(\mu') \frac{d\mu'}{\mu\sigma_n + \mu'\sigma_m} \quad (4.11a)$$

$$V_{mn}^k(\mu) = P_k(-\mu)\delta_{mn} + \frac{\mu}{2} \sum_{\ell} (-)^{\ell} \sum_{i,j=1}^N \int_0^1 P_k(\mu') U_{mi}^{\ell}(\mu') \frac{d\mu'}{\mu'\sigma_n + \mu\sigma_m} C_{ij}^{\ell} V_{jn}^{\ell}(\mu) \quad (4.12a)$$

in which form they are suitable for numerical solution by direct iteration.

Equations (4.11), (4.12) are only needed for the range  $k = 0, 1, 2, \dots, L$  where  $\ell = L$  is the last term retained in the sum over  $\ell$  in equation (4.1). If  $L = 0$  we will have simplified to the isotropic scattering model and equations (4.11), (4.12) then reduce to the equations for  $U(\mu)$ ,  $V(\mu)$  derived by Pahor and Shultis (1969) in their treatment of the isotropic scattering problem.

In the one group case ( $N = 1$ ) all the matrices collapse to scalars,  $U^{\ell}$  becomes equal to  $V^{\ell}$  and the equations (4.11), (4.12)

reduce to the equations (2.36) for the  $\phi_\ell(\mu)$  functions of Busbridge. If the scattering is isotropic these in turn reduce to the equation (2.10) for the isotropic scattering H-function.

Some integral properties of the matrices  $\underline{U}^\ell(\mu)$  and  $\underline{V}^\ell(\mu)$  are developed in appendix A.

#### 4.2.1 The Adjoint Equation

The adjoint transport equation for the source free half space  $0 \leq x < \infty$  is

$$\Sigma \underline{\phi}^*(x, \mu) - \mu \frac{\partial}{\partial x} \underline{\phi}^*(x, \mu) = \frac{1}{2} \sum_{\ell} P_{\ell}(\mu) \tilde{C}_{\ell} \int_0^1 P_{\ell}(\mu') \underline{\phi}^*(x, \mu') d\mu' \quad (4.13)$$

where  $\underline{\phi}^*(x, \mu)$  is the column vector of group angular adjoints, and here as elsewhere the tilde  $\sim$  is used to denote the result of transposing a matrix or vector. The specifiable boundary conditions in equation (4.13) are the values of  $\underline{\phi}^*(0, -\mu)$  when  $0 < \mu \leq 1$  and the limiting behaviour of  $\underline{\phi}^*(x, \mu)$  as  $x \rightarrow \infty$ .

The invariance principle which corresponds to equation (4.2) is expressed by

$$\underline{\phi}^*(x, \mu) = \frac{1}{2\mu} \int_0^1 \underline{S}^*(\mu, \mu') \underline{\phi}^*(x, -\mu') d\mu' \quad (4.14)$$

and after following through an analysis similar to that in section 4.2 it is found that

$$\underline{S}^*(\mu, \mu') = \tilde{\underline{S}}(\mu', \mu).$$



Evaluation of the adjoint reflection matrix  $\tilde{S}^*(\mu, \mu')$  thus involves no additional work after the regular reflection matrix has been determined.

As with the ordinary fluxes the various Legendre moments of the group angular adjoints at  $x = 0$  can now be calculated and from equation (4.14) these are found to be

$$\int_{-1}^1 P_\ell(\mu) \tilde{\phi}^*(0, \mu) d\mu = (-)^{\ell} \tilde{U}^{\ell}(\mu) E^m, \quad (4.15)$$

if the boundary conditions on equation (4.13) are taken as

$$\tilde{\phi}^*(0, -\mu) = E^m \delta(\mu - \mu_0)$$

$$\lim_{x \rightarrow \infty} \tilde{\phi}^*(x, \mu) = 0.$$

#### 4.2.2 Remarks about Uniqueness

Equation (4.15) supplies the physical interpretation of the matrices  $\tilde{U}^{\ell}(\mu)$  and by defining  $\tilde{U}^{\ell}(\mu)$  through this equation and  $\tilde{V}^{\ell}(\mu)$  through equation (4.10) we may expect by analogy with the one group problem that the question of uniqueness of the functions will be resolvable by appeal to these definitions.

That equations (4.11), (4.12) do not possess a unique solution is known for the isotropic scattering case. The nature of the non physical solutions is discussed by Pahor and Shultis (1969) who give additional constraints on the solutions

which are necessary "and in all likelihood...are sufficient" (Pahor and Shultis' words) to provide a unique definition. As with one group theory however, it is to be expected that when successive iterations are applied to equations (4.11), (4.12), the process when it converges will do so to a unique solution. A number of numerical examples to test this conjecture have been carried out with success in all trials, but it has to be recognised that this does no more than make plausible the truth of the conjecture. In an important special case discussed in Section 4.6 where the transfer matrices  $C^{\ell}$  are all lower triangular (that is the material in the half space does not allow upscattering) we shall be able to do rather better than rely on analogy.

#### 4.3 Evaluation of Differential Particle Current Albedos

With a reflection function calculable from equation (4.7a), it is possible to evaluate a number of different particle albedos. Following Selph (1968) we define for a semi infinite medium the group to group particle current albedo  $A_2(g_o, \theta_o, g)$  as the group  $g$  particle current reflected out at any angle due to a unit incident current of particles in group  $g_o$ , where the incident particles make an angle  $\theta_o$  with the normal to the medium.

To calculate  $A_2(g_o, \theta_o, g)$  the outward going current in group  $g$  is required when the incident angular fluxes are

$$\phi(0, \mu) = \frac{\delta(\mu - \mu_o)}{\mu_o} E_o^{g_o} \quad (\mu_o = \cos \theta_o)$$

and hence are non-zero only in group  $g_o$ . Now the inward currents

$$J_+ = \int_0^1 \mu \phi(0, \mu) d\mu = E_o^{g_o}$$

while the total currents are (from equation (4.10))

$$J = \int_{-1}^1 \mu \phi(0, \mu) d\mu = -V^1(\mu_o) \cdot E_o^{g_o}.$$

The outward currents  $J_-$  are given by

$$\begin{aligned} J_- &= J_+ - J \\ &= E_o^{g_o} + V^1(\mu_o) E_o^{g_o}. \end{aligned}$$

Thus explicitly

$$A_2(g_o, \theta_o, g) = \delta_{gg_o} + V_{gg_o}^1(\mu_o) \quad (4.16)$$

and this can be calculated numerically as discussed in Section 4.2.

If, however, the medium is being treated with the isotropic scattering model, then only the zero order matrices  $\underline{u}^0(\mu)$ ,  $\underline{v}^0(\mu)$  will be calculated in numerical work and the expression (4.16) will be valueless. We then calculate the

angular fluxes reflected from the medium by equation (4.2)

as

$$\phi(0, -\mu) = \frac{1}{2\mu\mu_0} S(\mu, \mu_0) E_0^{g_0}$$

and the reflected currents  $J_-$  are

$$\begin{aligned} J_- &= \int_0^1 \mu \phi(0, -\mu) d\mu \\ &= \int_0^1 \frac{S(\mu, \mu_0) E_0^{g_0}}{2\mu_0} d\mu. \end{aligned}$$

$$\begin{aligned} \text{Explicitly } A_2(g_0, \theta_0, g) &= [J_-]_g \\ &= \int_0^1 \frac{S_{gg_0}(\mu, \mu_0)}{2\mu_0} d\mu \\ &= \frac{1}{2} \int_0^1 \frac{\mu}{\mu_0 \sigma_g + \sigma_{g_0} \mu} \sum_{ij} U_{gi}^o(\mu) d\mu C_{ij}^o V_{jg_0}^o(\mu_0). \end{aligned}$$

Some elementary algebra and use of equation (4.12a) with  $L = 0$  allows this to be written

$$\begin{aligned} A_2(g_0, \theta_0, g) &= \delta_{gg_0} + \frac{1}{2\sigma_{g_0}} \sum_{ij} \int_0^1 U_{gi}^o(\mu) d\mu C_{ij}^o V_{jg_0}^o(\mu_0) \\ &\quad - \frac{\sigma_g}{\sigma_{g_0}} V_{gg_0}^o(\mu_0) \end{aligned} \quad (4.17)$$

with which numerical calculations are again simple.

#### 4.4 A Useful Relationship for Isotropic Scattering Theory

In the one group isotropic scattering model the relationship (2.18)

$$H(z)H(-z)T(z) = 1$$

was of fundamental importance in finding solutions to the standard one group transport problems discussed in Section 2.3. We shall be attempting to find solutions of the corresponding multi-group problems and for these the multigroup equivalent of equation (2.18) will be required.

When all group to group transfers are treated by isotropic scattering theory, equations (4.11), (4.12) reduce simply to the equations

$$\underline{\underline{U}}(\mu) = \underline{\underline{I}} + \frac{\mu}{2} \int_0^1 \underline{\underline{A}}(\mu, \mu') * [\underline{\underline{U}}(\mu) \underline{\underline{C}} \underline{\underline{V}}(\mu')] d\mu' \quad (4.18)$$

$$\underline{\underline{V}}(\mu) = \underline{\underline{I}} + \frac{\mu}{2} \int_0^1 \underline{\underline{A}}(\mu', \mu) * [\underline{\underline{U}}(\mu') \underline{\underline{C}} \underline{\underline{V}}(\mu)] d\mu' \quad (4.19)$$

the superscript zeros on the matrices  $\underline{\underline{U}}$ ,  $\underline{\underline{V}}$  and  $\underline{\underline{C}}$  being omitted.

Equations (4.18), (4.19) may be used to extend the domain of definition of the matrices to the complex  $z$ -plane cut along the negative real axis to the extent required to ensure the existence of all the integrals. For example  $\underline{\underline{U}}_{mn}(z)$  will be

defined in the plane cut from  $z = 0$  to  $z = -\sigma_m/\sigma_n$  whilst  $V_{mn}(z)$  will be defined if the plane is cut from  $z = 0$  to  $z = -\sigma_n/\sigma_m$  and both will be non singular in the region  $\text{Re}(z) > 0$ .

If now matrices  $\tilde{U}^\dagger(z)$ ,  $\tilde{V}^\dagger(z)$  are defined in the appropriately cut planes by the equations

$$U_{mn}^\dagger(z) = U_{mn}(z\sigma_m)$$

$$V_{mn}^\dagger(z) = U_{mn}(z\sigma_n)$$

then equation (4.18) may be written

$$\sum_i U_{mi}(\mu) \left\{ \delta_{in} - \frac{\mu}{2} \sum_j C_{ij} \int_0^1 \frac{V_{jn}(\mu')}{\mu\sigma_n + \mu'\sigma_m} d\mu' \right\} = \delta_{mn}$$

or, writing  $z = \mu/\sigma_m$

$$\sum_i U_{mi}^\dagger(z) \left\{ \delta_{in} - \frac{z}{2} \sum_j C_{ij} \int_0^1 \frac{V_{jn}(\mu')}{\mu' + z\sigma_n} d\mu' \right\} = \delta_{mn}.$$

Thus the inverse  $\tilde{U}^{\dagger^{-1}}(z)$  of  $\tilde{U}^\dagger(z)$  has elements

$$[\tilde{U}^{\dagger^{-1}}(z)]_{in} = \delta_{in} - \frac{z}{2} \sum_j C_{ij} \int_0^1 \frac{V_{jn}(\mu')}{\mu' + z\sigma_n} d\mu' \quad (4.20)$$

and

$$\tilde{U}^{\dagger^{-1}}(z) = \tilde{I} - \frac{z}{2} \tilde{C} \int_0^1 \tilde{V}(\mu') (z\tilde{\Sigma} + \mu' \tilde{I})^{-1} d\mu' \quad (4.21)$$

Similarly by writing  $z = \mu/\sigma_n$  it is possible to express equation (4.19) as

$$\sum_j \left\{ \delta_{mj} - \frac{z}{2} \sum_i \int_0^1 \frac{U_{mi}(\mu')}{\mu' + z\sigma_m} d\mu' C_{ij} \right\} V_{jn}(z) = \delta_{mn}$$

and the inverse of  $\tilde{V}^{\dagger}(z)$  is given by

$$[\tilde{V}^{\dagger^{-1}}(z)]_{mj} = \delta_{mj} - \frac{z}{2} \sum_i \int_0^1 \frac{U_{mi}(\mu')}{\mu' + z\sigma_m} d\mu' C_{ij} \quad (4.22)$$

or

$$\tilde{V}^{\dagger^{-1}}(z) = \tilde{I} - \frac{z}{2} \int_0^1 (z\Sigma + \mu' \tilde{I})^{-1} \tilde{U}(\mu') d\mu' \tilde{C}. \quad (4.23)$$

From equations (4.20), (4.22) it follows that

$$[\tilde{C}^{-1}(\tilde{I} - \tilde{U}^{\dagger^{-1}}(z))]_{jn} = \frac{z}{2} \int_0^1 \frac{V_{jn}(\mu')}{\mu' + z\sigma_n} d\mu'$$

$$[(\tilde{I} - \tilde{V}^{\dagger^{-1}}(z))\tilde{C}^{-1}]_{mi} = \frac{z}{2} \int_0^1 \frac{U_{mi}(\mu')}{\mu' + z\sigma_m} d\mu'.$$

Now consider

$$\mathcal{L} = [\tilde{V}^{\dagger^{-1}}(z)\tilde{C}^{-1}\tilde{U}^{\dagger^{-1}}(-z) - \tilde{V}^{\dagger^{-1}}(z)\tilde{C}^{-1} - \tilde{C}^{-1}\tilde{U}^{\dagger^{-1}}(-z) + \tilde{C}^{-1}]_{mn} \quad (4.24)$$

$$= [(\tilde{V}^{\dagger^{-1}}(z) - \tilde{I})\tilde{C}^{-1}(\tilde{U}^{\dagger^{-1}}(-z) - \tilde{I})]_{mn}$$

$$= \sum_{ij} -\frac{z}{2} \int_0^1 \frac{U_{mi}(\mu')}{\mu' + z\sigma_m} d\mu' C_{ij} \frac{z}{2} \int_0^1 \frac{V_{jn}(\mu'')}{\mu'' - z\sigma_n} d\mu''.$$

By a partial fraction expansion

$$\frac{z}{(\mu' + z\sigma_m)(\mu'' - z\sigma_n)} = \frac{1}{\mu''\sigma_m + \mu'\sigma_n} \left( \frac{\mu''}{\mu'' - z\sigma_n} - \frac{\mu'}{\mu' + z\sigma_m} \right)$$

$$\therefore \mathcal{L} = \frac{z}{2} \sum_{ij} \int_0^1 \frac{d\mu'}{\mu' + z\sigma_m} \frac{\mu'}{2} U_{mi}(\mu') C_{ij} \int_0^1 \frac{V_{jn}(\mu'')}{\mu'\sigma_n + \mu''\sigma_m} d\mu''$$

$$- \frac{z}{2} \sum_{ij} \int_0^1 d\mu'' \frac{\mu''}{2} \int_0^1 \frac{U_{mi}(\mu')}{\mu''\sigma_m + \mu'\sigma_n} d\mu' C_{ij} V_{jn}(\mu'') \frac{1}{\mu'' - z\sigma_n}$$

$$\begin{aligned}
&= \frac{z}{2} \int_0^1 \frac{d\mu'}{\mu' + z\sigma_m} \left\{ U_{mn}(\mu') - \delta_{mn} \right\} \\
&- \frac{z}{2} \int_0^1 \frac{d\mu''}{\mu'' - z\sigma_n} \left\{ V_{mn}(\mu'') - \delta_{mn} \right\} \\
&= [(\tilde{I} - \tilde{V}^{\dagger^{-1}}(z))\tilde{C}^{-1}]_{mn} - \delta_{mn} \frac{z}{2} \int_0^1 \frac{d\mu'}{\mu' + z\sigma_m} \\
&+ [\tilde{C}^{-1}(\tilde{I} - \tilde{U}^{\dagger^{-1}}(-z))]_{mn} + \delta_{mn} \frac{z}{2} \int_0^1 \frac{d\mu''}{\mu'' - z\sigma_n} \\
&= [\tilde{C}^{-1}]_{mn} - [(\tilde{V}^{\dagger^{-1}}(z))\tilde{C}^{-1}]_{mn} + [\tilde{C}^{-1}]_{mn} - [\tilde{C}^{-1}(\tilde{U}^{\dagger^{-1}}(-z))]_{mn} \\
&- \frac{z}{2} \delta_{mn} \log \left| \frac{1+z\sigma_m}{z\sigma_m} \cdot \frac{z\sigma_n}{z\sigma_n - 1} \right|.
\end{aligned}$$

Because the Kronecker delta is only non zero when  $m = n$  the last term in  $\mathcal{L}$  can be replaced by

$$- \frac{z}{2} \delta_{mn} \log \left| \frac{z\sigma_m + 1}{z\sigma_m - 1} \right|.$$

Finally when this final form for  $\mathcal{L}$  is equated to that originally given by equation (4.24) most terms cancel out leaving

$$[(\tilde{V}^{\dagger^{-1}}(z))\tilde{C}^{-1}(\tilde{U}^{\dagger^{-1}}(-z))]_{mn} = [\tilde{C}^{-1}]_{mn} - \frac{z}{2} \delta_{mn} \log \left| \frac{z\sigma_m + 1}{z\sigma_m - 1} \right|. \quad (4.25)$$

If now by analogy with equation (2.18) the matrix  $T(z)$  is defined as

$$[T(z)]_{mn} = \delta_{mn} - C_{mn} \frac{z}{2} \log \left| \frac{z\sigma_m + 1}{z\sigma_m - 1} \right| \quad (4.26)$$



equation (4.25) may be written

$$\tilde{V}^{-1}(z) \tilde{C}^{-1} \tilde{U}^{-1}(-z) = \tilde{T}(z) \tilde{C}^{-1}$$

so that

$$\left. \begin{aligned} \tilde{T}(z) &= \tilde{V}^{-1}(z) \tilde{C}^{-1} \tilde{U}^{-1}(-z) \tilde{C} \\ \text{or} \quad \tilde{T}(z) &= \tilde{V}^{-1}(-z) \tilde{C}^{-1} \tilde{U}^{-1}(z) \tilde{C} \end{aligned} \right\} \quad (4.27)$$

since  $\tilde{T}(z)$  is an even function of  $z$ . In the one group problem, equation (4.27) collapses to equation (2.18) as expected.

It is well known (see for example Yoshimura and Katsuragi, 1968) that the zeroes of  $\tilde{T}(z)$ , that is those values of  $z$  for which the determinant of  $\tilde{T}$  vanishes, occur in pairs  $\pm z_i$  and that the real positive zeroes are the material diffusion lengths whose reciprocals we denote by  $\kappa_i$ . For a general transfer matrix  $\tilde{C}$  there seems to be no a priori reason why any  $z_i$  should be real. However it is argued on physical grounds that for subcritical materials the dominant zero  $z_0$ , i.e. that  $z_i$  with largest real part, will be real. The corresponding  $\kappa_0$  is also then real and, far from the source, all angular fluxes will have a spatial variation of the form  $\exp(-\kappa_0 x)$ .

From the first of equations (4.27) it follows that for each zero  $z_i$  with positive real part either  $\tilde{V}^{-1}(z_i)$  or  $\tilde{U}^{-1}(-z_i)$  must have a pole, and from the second equation (4.27) it follows also that either  $\tilde{V}^{-1}(-z_i)$  or  $\tilde{U}^{-1}(z_i)$  must have a pole.

Since  $\tilde{U}^\dagger(z)$  and  $\tilde{V}^\dagger(z)$  are known to be free from poles in the half plane  $\operatorname{Re}(z) > 0$  it is clear that the poles will be in  $\tilde{U}^\dagger(-z_i)$  and  $\tilde{V}^\dagger(-z_i)$ .

#### 4.5 Analytic Solutions for Two Multigroup Transport Problems

In this section an attempt is made to find analytic solutions to the multigroup equivalents of the two problems studied in Section 2.3 - the albedo problem and the Milne problem. The problems are studied in the isotropic scattering model only but even then with only partial success. For anisotropic scattering problems numerical solution seems to be the only feasible technique and this is taken up in a later section.

##### 4.5.1 The Multigroup Albedo Problem

The problem chosen here is to find the asymptotic solution of the multigroup transport equation

$$\Sigma \tilde{\phi}(x, \pm\mu) \pm \mu \frac{\partial}{\partial x} \tilde{\phi}(x, \pm\mu) = \frac{1}{2} \tilde{C} \int_{-1}^1 \tilde{\phi}(x, \mu') d\mu' \quad (4.28)$$

$$\text{with } \tilde{\phi}(0, \mu) = \delta(\mu - \mu_0) E^n, \quad 0 < \mu, \mu_0 \leq 1 \quad (4.29)$$

$$\text{and } \lim_{x \rightarrow \infty} \tilde{\phi}(x, \pm\mu) = 0$$

and where  $\tilde{C}$  has been written for the isotropic transfer matrix  $\tilde{C}^0$ .

The simple boundary conditions (4.29) represent the physical situation where a beam of neutrons in group  $n$  enters the medium at  $x = 0$  making an angle  $\cos^{-1}(\mu_0)$  with the positive  $x$  axis. As in Section 2.3 this simple boundary condition is selected because the solution of the simple problem can be used to generate solutions of the albedo problem with any other set of initial angular fluxes.

The emerging angular fluxes have already been calculated in section 4.4 as

$$\bar{\phi}(0, -\mu) = \frac{1}{2\mu} S(\mu, \mu_0) E^n,$$

so that for group  $m$

$$\begin{aligned} \phi_m(0, +\mu) &= \delta_{mn} \delta(\mu - \mu_0) \\ \phi_m(0, -\mu) &= \frac{1}{2\mu} S_{mn}(\mu, \mu_0) \\ &= \frac{1}{2} \frac{\mu_0}{\mu \sigma_n + \mu_0 \sigma_m} \sum_{ij} U_{mi}(\mu) C_{ij} V_{jn}(\mu_0). \end{aligned}$$

Again the initial value of the angular fluxes are known so that a Laplace Transform treatment of equation (4.28) is possible. The Laplace Transform of the group  $m$  angular flux is

$$\bar{\phi}_m(p, \mu) = \int_0^{\infty} e^{-px} \phi_m(x, \mu) dx,$$

whilst the group  $m$  scalar flux

$$\phi_m(x) = \int_{-1}^1 \phi_m(x, \mu') d\mu'$$

has Laplace Transform

$$\begin{aligned}\bar{\phi}_m(p) &= \int_{-1}^1 \bar{\phi}_m(p, \mu') d\mu' \\ &= \int_0^\infty e^{-px} \phi_m(x) dx.\end{aligned}$$

Taking the Laplace Transform of equation (4.28) in group m

$$\begin{aligned}\sigma_m \bar{\phi}_m(p, \mu) + \mu p \bar{\phi}_m(p, \mu) \\ - \mu \phi_m(0, \mu) = \frac{1}{2} \sum_j C_{mj} \bar{\phi}_j(p)\end{aligned}$$

and  $\sigma_m \bar{\phi}_m(p, -\mu) - \mu p \bar{\phi}_m(p, -\mu)$

$$+ \mu \phi_m(0, -\mu) = \frac{1}{2} \sum_j C_{mj} \bar{\phi}_j(p).$$

When the initial values for the angular fluxes are inserted these equations become

$$\begin{aligned}\bar{\phi}_m(p, \mu) &= \frac{\mu \delta_{mn}}{\sigma_m + \mu p} \delta(\mu - \mu_o) + \frac{1}{2} \frac{1}{\sigma_m + \mu p} \sum_j C_{mj} \bar{\phi}_j(p), \\ \bar{\phi}_m(p, -\mu) &= \frac{-\mu \mu_o}{2(\sigma_m - \mu p)} \sum_{ij} \frac{U_{mi}(\mu) C_{ij} V_{jn}(\mu_o)}{\mu \sigma_n + \mu_o \sigma_m} \\ &+ \frac{1}{2} \frac{1}{\sigma_m - \mu p} \sum_j C_{mj} \bar{\phi}_j(p).\end{aligned}$$

To obtain an equation involving only the transform of the scalar fluxes these last equations have to be integrated

over the range  $0 \leq \mu \leq 1$  and the results added together.

From the results

$$\frac{1}{2} \int_0^1 \frac{d\mu}{\sigma_m + \mu p} + \frac{1}{2} \int_0^1 \frac{d\mu}{\sigma_m - \mu p} = \frac{1}{2p} \log \left| \frac{\sigma_m + p}{\sigma_m - p} \right|$$

and 
$$\int \frac{\mu \delta_{mn}}{\sigma_m + \mu p} \delta(\mu - \mu_o) d\mu = \frac{\mu_o \delta_{mn}}{\sigma_n + \mu_o p},$$

it follows that

$$\begin{aligned} \bar{\phi}_m(p) &= \frac{\mu_o \delta_{mn}}{\sigma_n + \mu_o p} + \frac{1}{2p} \log \left| \frac{\sigma_m + p}{\sigma_m - p} \right| \sum_j C_{mj} \bar{\phi}_j(p) \\ &\quad - \frac{\mu_o}{2} \sum_{ij} \int_0^1 \frac{\mu U_{mi}(\mu)}{(\mu \sigma_n + \mu_o \sigma_m)(\sigma_m - \mu p)} d\mu C_{ij} V_{jn}(\mu_o). \end{aligned}$$

After using the partial fraction expansion

$$\frac{\mu}{(\mu \sigma_n + \mu_o \sigma_m)(\sigma_m - \mu p)} = \frac{1}{(\sigma_n + \mu_o p)} \left\{ \frac{1}{\sigma_m - \mu p} - \frac{\mu_o}{\mu \sigma_n + \mu_o \sigma_m} \right\}$$

and collecting terms we obtain

$$\begin{aligned} &\sum_j \left\{ \delta_{mj} - \frac{C_{mj}}{2p} \log \left| \frac{\sigma_m + p}{\sigma_m - p} \right| \right\} \bar{\phi}_j(p) \\ &= \frac{\mu_o}{\sigma_n + \mu_o p} \left\{ \delta_{mn} + \frac{\mu_o}{2} \sum_{ij} \int_0^1 \frac{U_{mi}(\mu)}{\mu \sigma_n + \mu_o \sigma_m} d\mu C_{ij} V_{jn}(\mu_o) \right. \\ &\quad \left. - \frac{1}{2} \sum_{ij} \int_0^1 \frac{U_{mi}(\mu)}{\sigma_m - \mu p} d\mu C_{ij} V_{jn}(\mu_o) \right\}. \end{aligned}$$

From equations (4.19) and (4.26) it follows that this may be written

$$\begin{aligned} \sum_j T_{mj} \left(\frac{1}{p}\right) \bar{\phi}_j(p) &= \frac{\mu_o}{\sigma_n + \mu_o p} \left\{ v_{mn}(\mu_o) - \frac{1}{2} \sum_{ij} \int \frac{U_{mi}(\mu)}{\sigma_m - \mu p} d\mu C_{ij} v_{jn}(\mu_o) \right\} \\ &= \frac{\mu_o}{\sigma_n + \mu_o p} \sum_j \left\{ \delta_{mj} - \frac{1}{2} \left(-\frac{1}{p}\right) \sum_i \int \frac{U_{mi}(\mu')}{\mu' - \sigma_m} d\mu' C_{ij} \right\} v_{jn}(\mu_o) \end{aligned}$$

or from equation (4.22)

$$\sum_j T_{mj} \left(\frac{1}{p}\right) \bar{\phi}_j(p) = \frac{\mu_o}{\sigma_n + \mu_o p} \sum_j \left( V^{-1} \left(-\frac{1}{p}\right) \right)_{mj} v_{jn}(\mu_o).$$

This has the matrix form

$$\tilde{T} \left(\frac{1}{p}\right) \tilde{\bar{\phi}}(p) = \frac{\mu_o}{\sigma_n + \mu_o p} \tilde{V}^{-1} \left(-\frac{1}{p}\right) \tilde{V}(\mu_o) \tilde{E}^n \quad (4.30)$$

and from the relation (4.27) can be written

$$\tilde{\bar{\phi}}(p) = \frac{\mu_o}{(\sigma_n + \mu_o p)} \tilde{C}^{-1} \tilde{U}^T \left(\frac{1}{p}\right) \tilde{C} \tilde{V}(\mu_o) \tilde{E}^n. \quad (4.31)$$

The scalar flux vector is then to be found by inverting the Laplace Transform. The form (4.31) shows that the singularities in  $\tilde{\bar{\phi}}(p)$  are in the negative half plane and will come from the singularities in  $\tilde{U}^T \left(\frac{1}{p}\right)$  and from the point  $p = -\sigma_n / \mu_o$ . The asymptotic flux for large  $x$ , in which the real interest lies, will come from the pole with smallest real part (say  $p = -\kappa$ ) and the transform may formally be inverted

with the aid of the inversion theorem to give

$$\phi_{asy}(x) = \left( \frac{\mu_0}{\sigma_n - \mu_0 \kappa_0} \right) \lim_{p \rightarrow -\kappa_0} \left\{ (p + \kappa_0)^{-1} C^{-1} U \left( \frac{1}{p} \right) C V(\mu_0) E^n \right\} e^{-\kappa_0 x}. \quad (4.32)$$

The angular fluxes in this asymptotic region are then found from the transport equation (4.28) to be

$$\phi(x, \pm\mu) = \frac{1}{2} (\Sigma \pm \mu \kappa_0 I)^{-1} C \phi_{asy}(x)$$

and it may be said then that equation (4.32) gives the required asymptotic solution.

There seems to be no analytical procedure for evaluating the limit in equation (4.32). Use of this equation for finding numerical solutions will then require that the limit be sought numerically.

#### 4.5.2 The Multigroup Milne Problem

With this problem solutions of the transport equation (4.28) are sought when there is no inward flow of neutrons at  $x = 0$ , the neutrons in the half space  $x > 0$  being supplied from some source at infinity, so that an asymptotic flux distribution varying like  $e^{\kappa x}$  is set up for large  $x$ . Formally there are as many Milne problems as there are positive real values for  $\kappa$  for which  $|T(\frac{1}{\kappa})| = 0$ . We restrict our attention to the Milne problem associated with the dominant  $\kappa$ .

Since there will, in this problem, be neutrons which make their first crossing of any  $x$  plane travelling in directions with negative  $\mu$ , an additional term has to be added to the right hand side of equation (4.2) to include these neutrons. The modified equation then reads

$$\dot{\phi}(x, -\mu) = \dot{\phi}_x(x, -\mu) + \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \dot{\phi}(x, +\mu') d\mu' \quad (4.33)$$

and by exactly the argument used in Section 2

$$\dot{\phi}_x(x, -\mu) = e^{\kappa x} \dot{\phi}(0, -\mu).$$

The evaluation of the emerging angular fluxes is the first task and to do so we differentiate equation (4.33) with respect to  $x$ , insert the now known form for  $\dot{\phi}_x(x, -\mu)$  and then set  $x = 0$  to obtain

$$\dot{\phi}(0, -\mu) = \kappa \dot{\phi}(0, -\mu) + \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \dot{\phi}(0, +\mu') d\mu'.$$

From the transport equation (4.28)

$$\begin{aligned} \dot{\phi}(0, \mu) &= -\frac{1}{\mu} \Sigma \dot{\phi}(0, \mu) + \frac{1}{2\mu} C \int_0^1 \dot{\phi}(0, \mu') d\mu' + \frac{1}{2\mu} C \int_0^1 \dot{\phi}(0, -\mu') d\mu' \\ &= \frac{1}{2\mu} C \int_0^1 \dot{\phi}(0, -\mu') d\mu' \end{aligned}$$

since  $\dot{\phi}(0, +\mu) = 0$ ,

while  $\dot{\phi}(0, -\mu) = \frac{1}{\mu} \Sigma \dot{\phi}(0, -\mu) - \frac{1}{2\mu} C \int_0^1 \dot{\phi}(0, -\mu') d\mu'.$



Eliminating the derivatives between these last three equations

$$\text{gives } (\frac{1}{\mu} \Sigma - \kappa I) \phi(0, \mu) = \frac{1}{2\mu} \left( I + \int_0^1 S(\mu, \mu') \frac{d\mu'}{2\mu'} \right) C \int_0^1 \phi(0, -\mu') d\mu'$$

and this may be written, after using equation (4.8) which defines the matrix  $U$ , as

$$\phi(0, -\mu) = \frac{1}{2} (\Sigma - \kappa \mu I)^{-1} U(\mu) C \int_0^1 \phi(0, -\mu') d\mu'. \quad (4.34)$$

Equation (4.34) formally determines the emerging distributions, and may in fact be used to compute them numerically.

If it is integrated over the range  $0 \leq \mu \leq 1$  it may be written

$$\left\{ I - \frac{1}{2} \int_0^1 (\Sigma - \kappa \mu I)^{-1} U(\mu) d\mu C \right\} \int_0^1 \phi(0, -\mu') d\mu' = 0 \quad (4.35)$$

or from equation (4.23)

$$V^{-1} \left( -\frac{1}{\kappa} \right) C \int_0^1 \phi(0, -\mu') d\mu' = 0$$

so that  $\int_0^1 \phi(0, -\mu') d\mu'$ , the vector of scalar fluxes at the boundary  $x = 0$ , is that eigen vector of the matrix  $V^{-1} \left( -\frac{1}{\kappa} \right) C$  corresponding to its zero eigen value. This is easily computed and equation (4.34) may then be used to determine the angular distributions.

With the angular fluxes at the boundary now known we again use the Laplace Transform method for solution of equation (4.28). The analysis is similar to that used in the previous

section and it is found that the transformed equation for the group scalar fluxes can be written

$$\begin{aligned} \tilde{T}\left(\frac{1}{p}\right)\tilde{\phi}(p) &= -\int_0^1 \mu (\tilde{\Sigma} - \mu p \tilde{I})^{-1} \tilde{\phi}(0, -\mu) d\mu \\ &+ \int_0^1 \mu (\tilde{\Sigma} + \mu p \tilde{I})^{-1} \tilde{\phi}(0, +\mu) d\mu \end{aligned} \quad (4.36)$$

with the last integral zero because no neutrons enter the half space at  $x = 0$ . We now simplify by substituting equation (4.34) for the emergent angular fluxes and use of the partial fraction expansion

$$\begin{aligned} &-\mu (\tilde{\Sigma} - \mu p \tilde{I})^{-1} (\tilde{\Sigma} - \kappa \mu \tilde{I})^{-1} \\ &= \frac{1}{p - \kappa} \left\{ (\tilde{\Sigma} - \kappa \mu \tilde{I})^{-1} - (\tilde{\Sigma} - \mu p \tilde{I})^{-1} \right\}, \end{aligned}$$

which expansion is elementary because all the matrices used are diagonal. These manipulations result in the equation

$$\begin{aligned} \tilde{T}\left(\frac{1}{p}\right)\tilde{\phi}(p) &= \frac{1}{p - \kappa} \left\{ \frac{1}{2} \int_0^1 (\tilde{\Sigma} - \kappa \mu \tilde{I})^{-1} \tilde{U}(\mu) d\mu \quad \tilde{C} \int_0^1 \tilde{\phi}(0, -\mu') d\mu' \right. \\ &\quad \left. - \frac{1}{2} \int_0^1 (\tilde{\Sigma} - \mu p \tilde{I})^{-1} \tilde{U}(\mu) d\mu \quad \tilde{C} \int_0^1 \tilde{\phi}(0, -\mu') d\mu' \right\}. \end{aligned}$$

Successive use of equations (4.35) and (4.23) reduces this to

$$\tilde{T}\left(\frac{1}{p}\right)\tilde{\phi}(p) = \frac{1}{p - \kappa} \tilde{V}^{-1} \left( -\frac{1}{p} \right) \int_0^1 \tilde{\phi}(0, -\mu') d\mu'$$

and from the relation (4.27) it follows that

$$\bar{\phi}(p) = \frac{1}{p-\kappa} \tilde{C}^{-1} \tilde{U}^{\dagger} \left( \frac{1}{p} \right) \tilde{C} \int_0^1 \phi(0, -\mu') d\mu' . \quad (4.37)$$

The asymptotic part of the flux vector is composed of two parts, one proportional to  $e^{\kappa x}$  and coming from the residue at  $p = \kappa$  introduced by the factor  $\frac{1}{p-\kappa}$  in  $\bar{\phi}(p)$ . The other contribution, proportional to  $e^{-\kappa x}$ , arises from the residue at  $p = -\kappa$  introduced by the pole of  $\tilde{U}^{\dagger}(\frac{1}{p})$  at this point. Thus

$$\phi_{asy}(x) = \tilde{A} e^{\kappa x} + \tilde{B} e^{-\kappa x}$$

and from the inversion theorem

$$\left. \begin{aligned} \tilde{A} &= \tilde{C}^{-1} \tilde{U}^{\dagger} \left( \frac{1}{\kappa} \right) \tilde{C} \int_0^1 \phi(0, -\mu') d\mu' \\ \text{and } \tilde{B} &= -\frac{1}{2\kappa} \lim_{p \rightarrow -\kappa} (p+\kappa) \tilde{C}^{-1} \tilde{U}^{\dagger} \left( \frac{1}{p} \right) \tilde{C} \int_0^1 \phi(0, -\mu') d\mu' . \end{aligned} \right\} \quad (4.38)$$

From these we may calculate the extrapolation length for group

$$m \text{ say, as } (x_0)_m = \frac{+1}{2\kappa} \log \left| \frac{\tilde{A}_m}{-\tilde{B}_m} \right|$$

while the ratio in group  $m$  of the asymptotic flux to the true flux is

$$\frac{\phi_{masy}(x)}{\phi_m(x)} = \frac{\tilde{A}_m + \tilde{B}_m}{1 - \int_0^1 \phi_m(0, -\mu') d\mu'}$$

As for the albedo problem we can find no general solution to the problem of evaluating the limit  $\lim_{p \rightarrow \kappa^-} U^{\dagger}(\frac{1}{p})$  analytically and must be content for the moment to leave the solution at the stage defined by equations (4.37), (4.38).

#### 4.6      Slowing Down Media

The most useful application of the multigroup Chandrasekhar method is likely to be in deep penetration calculations associated with shielding problems. For such calculations the material in which the neutrons move can be treated as one in which upscattering is impossible and this of course places a major restriction on the form of the transfer matrices  $C^{\ell}$ . Fortunately it happens that the restriction is such as to make numerical calculations much simpler.

Let us therefore consider the half space  $0 \leq x < \infty$  to be occupied by a purely down scattering material so that when the groups are numbered sequentially in lethargy with group 1 the lowest lethargy group, the restriction is that

$$C_{ij}^{\ell} = 0 \quad \text{for } i < j, \quad \ell = 0, 1, \dots,$$

and the matrices  $C^{\ell}$  are all lower triangular. Since no neutrons are then able to reach a group numbered lower than that in which they entered the medium the reflection matrix  $S(\mu, \mu')$  is also lower triangular and from equations (4.8), (4.9) all matrices

$U^\ell(\mu), V^\ell(\mu)$  are lower triangular. This means that the ranges over which the summations extend in equations (4.7a), (4.11a), (4.12a) are considerably reduced, and the equations become for  $m \geq n$

$$S_{mn}(\mu, \mu_0) = \frac{\mu \mu_0}{\mu \sigma_n + \mu_0 \sigma_m} \sum_{\ell} (-)^{\ell} \sum_{i=n}^m \sum_{j=n}^i U_{mi}^{\ell}(\mu) C_{ij}^{\ell} V_{jn}^{\ell}(\mu_0) \quad (4.39)$$

$$U_{mn}^k(\mu) = P_k(-\mu) \delta_{mn} + \frac{\mu}{2} \sum_{\ell} (-)^{\ell} \sum_{i=n}^m U_{mi}^{\ell}(\mu) \sum_{j=n}^i C_{ij}^{\ell} \int_0^1 P_k(\mu') V_{jn}^{\ell}(\mu') \frac{d\mu'}{\mu \sigma_n + \mu' \sigma_m} \quad (4.40)$$

$$V_{mn}^k(\mu) = P_k(-\mu) \delta_{mn} + \frac{\mu}{2} \sum_{\ell} (-)^{\ell} \sum_{i=n}^m \int_0^1 P_k(\mu') U_{mi}^{\ell}(\mu') \frac{d\mu'}{(\mu' \sigma_n + \mu \sigma_m)} \sum_{j=n}^i C_{ij}^{\ell} V_{jn}^{\ell}(\mu) . \quad (4.41)$$

When  $n = m$  we will be computing the elements of the matrices on the principal diagonal and sums over  $i, j$  in these last three equations comprise only a single term. In addition the elements  $U_{mm}^k(\mu), V_{mm}^k(\mu)$  become equal and satisfy

$$U_{mm}^k(\mu) = P_k(-\mu) + \frac{\mu}{2} \sum_{\ell} (-)^{\ell} U_{mm}^{\ell}(\mu) \frac{C_{mm}^{\ell}}{\sigma_m} \int P_k(\mu') \frac{U_{mm}(\mu')}{\mu + \mu'} d\mu'$$

which is simply equation (2.36), the equation satisfied by Busbridge's

$\phi_\ell(\mu)$  functions. At the same time the component  $S_{mm}(\mu, \mu_0)$  of the reflection matrix becomes

$$S_{mm}(\mu, \mu_0) = \frac{\mu\mu_0}{\mu+\mu_0} \sum_{\ell} (-)^{\ell} U_{mm}^{\ell}(\mu) \frac{C_{mm}^{\ell}}{\sigma_m} U_{mm}^{\ell}(\mu_0) \quad (4.42)$$

which is essentially equation (2.35), the equation for the one group anisotropic scattering reflection function.

#### 4.6.1 The Uniqueness Question

In one group the definition of  $\phi_\ell(\mu)$  functions as the various Legendre polynomial moments of the angular flux on the boundary is sufficient to define them uniquely and, in addition, it is known that the method of repeated substitution when it converges, does so to these unique solutions. For the present multigroup slowing down problem this means that the question of uniqueness of the diagonal elements of the  $U^{\ell}(\mu)$ ,  $V^{\ell}(\mu)$  matrices and of the reflection matrix is resolved satisfactorily. With these diagonal elements uniquely defined it is then necessary to examine the matrix elements in the immediate neighbourhood of the leading diagonal. For these elements the defining equation may be written

$$\begin{aligned} U_{n+1,n}^k(\mu) &= \sum_{\ell} \alpha_{\ell} \int_0^1 \frac{P_{\ell}(\mu') V_{n+1,n}^{\ell}(\mu')}{\mu\sigma_n + \mu'\sigma_{n+1}} d\mu' \\ &+ \sum_{\ell} \beta_{\ell}^k U_{n+1,n}^{\ell}(\mu) \\ &+ \gamma^k, \quad k = 0, 1, \dots, \end{aligned} \quad (4.43)$$

$$\begin{aligned}
V_{n+1,n}^k(\mu) &= \sum_{\ell} \xi_{\ell} \int_0^1 \frac{P_k(\mu') U_{n+1,n}^{\ell}(\mu')}{\mu' \sigma_n + \mu \sigma_{n+1}} d\mu' \\
&+ \sum_{\ell} \eta_{\ell}^k V_{n+1,n}^{\ell}(\mu) \\
&+ \zeta^k, \quad k = 0, 1, \dots \quad (4.44)
\end{aligned}$$

Here

$$\begin{aligned}
\alpha_{\ell} &= (-)^{\ell} \frac{\mu}{2} U_{n+1,n+1}^{\ell}(\mu) C_{n+1,n+1}^{\ell}, \\
\beta_{\ell}^k &= (-)^{\ell} \frac{\mu}{2} C_{n,n}^{\ell} \int_0^1 \frac{P_k(\mu') V_{n,n}^{\ell}(\mu')}{\mu \sigma_n + \mu' \sigma_{n+1}} d\mu', \\
\gamma^k &= \frac{\mu}{2} \sum_{\ell} (-)^{\ell} U_{n+1,n+1}^{\ell}(\mu) C_{n+1,n}^{\ell} \int_0^1 \frac{P_k(\mu') V_{n,n}^{\ell}(\mu')}{\mu \sigma_n + \mu' \sigma_{n+1}} d\mu', \\
\xi_{\ell} &= (-)^{\ell} \frac{\mu}{2} C_{nn}^{\ell} V_{nn}^{\ell}(\mu), \\
\eta_{\ell}^k &= (-)^{\ell} \frac{\mu}{2} C_{n+1,n+1}^{\ell} \int_0^1 \frac{P_k(\mu') U_{n+1,n+1}^{\ell}(\mu')}{\mu' \sigma_n + \mu \sigma_{n+1}} d\mu', \\
\zeta^k &= \frac{\mu}{2} \sum_{\ell} (-)^{\ell} \int_0^1 \frac{P_k(\mu') U_{n+1,n+1}^{\ell}(\mu')}{\mu' \sigma_n + \mu \sigma_{n+1}} d\mu' C_{n+1,n}^{\ell} V_{n+1,n}^{\ell}(\mu),
\end{aligned}$$

and all of these coefficients are explicit functions of the diagonal elements  $U_{n,n}^{\ell}(\mu)$ ,  $V_{n,n}^{\ell}(\mu)$  which have already been determined. The equations (4.43), (4.44) are a set of linear inhomogeneous Fredholm equations of the second kind. They therefore have a unique solution (Whittaker and Watson, 1927),

if and only if the corresponding homogeneous equations only have the trivial solution zero. If the  $\mu$  variation of the various functions is treated by a discrete ordinate representation - as it will be in numerical work - equations (4.43), (4.44) will become a set of linear algebraic equations for which the uniqueness question can be resolved by examining the coefficient determinant for the equations.

In practice a standard routine for solution of sets of linear equations will certainly be used (say the Gauss Jordan method) and these routinely test the determinant. Because the coefficients in equations (4.43), (4.44) depend on the group cross sections it may reasonably be claimed that this determinant will not always be zero and that therefore the equations will have unique solutions for at least some cross sections. Attempts to establish conditions on the cross sections which will ensure uniqueness of the solutions have been unsuccessful but the candidate suspects that the solutions will be unique provided the absorption cross sections are such that the material is subcritical. If the terms  $U_{n+1,n}(\mu)$ ,  $V_{n+1,n}(\mu)$  are found to be uniquely determined, attention must be turned to the terms in the next diagonal, and their uniqueness established. Proceeding in this fashion along the various diagonals, equations (4.40), (4.41) for the terms  $U_{n+r,n}^{\ell}(\mu)$ ,  $V_{n+r,n}^{\ell}(\mu)$  are again found to be a set



of linear inhomogeneous Fredholm equations with coefficients depending on the various group cross sections and on elements of the  $\tilde{U}^{\ell}(\mu)$   $\tilde{V}^{\ell}(\mu)$  matrices which have already been evaluated. Again when a discrete angle representation is adopted for the angular variation these equations become a set of linear inhomogeneous equations and the same test for uniqueness applies as has been discussed for the terms  $U_{n+1,n}^{\ell}(\mu)$ ,  $V_{n+1,n}^{\ell}(\mu)$ .

With a discrete angle representation then, the uniqueness question is no problem - if the equations can be solved the solution is unique.

#### 4.6.2 Numerical Evaluation of the $\tilde{U}^{\ell}(\mu)\tilde{V}^{\ell}(\mu)$ Matrices

As well as providing a base for the (non-rigorous) uniqueness proof sketched above this strategy for determining the various matrix elements in pairs is a successful one in practice. A computer programme using this strategy has been written for the IBM-360/50 computer and run successfully for a variety of materials ranging in density and composition from dry air to a light concrete. Computing times vary, of course, with the complexity of the problem but as rough indication we remark that for a ten group problem with  $P_3$  scattering where the  $\mu$  range (0,1) was represented by eight quadrature points evaluation of all the matrix elements takes something less than

ten minutes. With  $P_1$  scattering and two quadrature points in  $0 < \mu \leq 1$  about twenty seconds time is required for solution.

For the solution of equations (4.11), (4.12) in general, an efficient strategy has not yet been found nor is it yet possible to make any comment about the question of the uniqueness of solutions to these equations. A solution can however be attempted by repeated substitution methods and in each of the few examples tested the attempt was successful. The solution found was physically meaningful in the sense that when a reflection matrix computed from equation (4.7) was used to evaluate the group angular fluxes reflected from a semi infinite medium, these were found to be in excellent agreement with the angular fluxes reflected from a very thick homogeneous slab as calculated by conventional  $S_N$  methods.

#### 4.7 Numerical Solution of the Albedo Problem

In section (4.5) an attempt was made (with limited success) to generate an analytic solution to the albedo problem for a semi infinite medium with isotropic scattering in all groups. It was found necessary to leave this solution at the stage where a limiting process had to be carried out by numerical means to obtain the asymptotic form of the solution as  $x \rightarrow \infty$ . We now develop a procedure for direct numerical solution of the problem. The procedure, which is able to handle arbitrarily

anisotropic scattering and can develop the numerical solution for all values of  $x$  small or large, uses a discrete ordinate representation for the  $\mu$  variation of the angular fluxes so that integrals over  $\mu$  are evaluated as weighted sums.

It is of course well known that numerical solution of the problem with the discrete ordinate approximation can (at least conceptually) be tackled by conventional  $S_N$  codes. The semi infinite medium can be approximated by a very thick slab with a free boundary condition at the face remote from the source, and the fluxes in the semi infinite medium are well approximated by those in the finite slab except at points near to the free boundary. The difficulties with this conventional treatment have already been pointed out in Section 1, all being associated with the need for many iterations to converge the fluxes at the various mesh points.

If the transport equation (4.1) is written in slightly modified form for  $0 < \mu < 1$  as

$$\begin{aligned} \Sigma \phi(x, \mu) + \mu \frac{\partial}{\partial x} \phi(x, \mu) &= \frac{1}{2} \sum_{\ell} P_{\ell}(\mu) C^{\ell} \int_0^1 P_{\ell}(\mu') \phi(x, \mu') d\mu' \\ &+ \frac{1}{2} \sum_{\ell} P_{\ell}(\mu) C^{\ell} \int_0^1 P_{\ell}(-\mu') \phi(x, -\mu') d\mu' \end{aligned}$$

it can be seen that the difficulty of solution by conventional

methods is associated with the apparent need for knowledge of the angular fluxes with  $\mu$  negative in order to solve this equation for positive  $\mu$ , while the  $\mu$ -negative fluxes are themselves determined by  $\mu$ -positive fluxes - hence the need for iterations at each mesh point.

The method which we now develop obviates this need for iteration by using equation (4.2) to eliminate the  $\mu$ -negative fluxes from the transport equation which becomes

$$\begin{aligned} \Sigma \phi(x, \mu) + \mu \frac{\partial}{\partial x} \phi(x, \mu) &= \frac{1}{2} \sum_{\ell} P_{\ell}(\mu) C^{\ell} \int_0^1 P_{\ell}(\mu') \phi(x, \mu') d\mu' \\ &+ \frac{1}{2} \sum_{\ell} P_{\ell}(\mu) C^{\ell} \int_0^1 P_{\ell}(-\mu') \frac{1}{2\mu} \int_0^1 S(\mu' \mu'') \phi(x, \mu'') d\mu'' d\mu' \\ &= \frac{1}{2} \sum_{\ell} P_{\ell}(-\mu) C^{\ell} \int_0^1 V^{\ell}(\mu') \phi(x, \mu') d\mu' \end{aligned}$$

from equation (4.9). If the matrix  $B(\mu, \mu')$  is defined as

$$B(\mu, \mu') = \frac{1}{2\mu} \sum_{\ell} P_{\ell}(-\mu) C^{\ell} V^{\ell}(\mu') - \frac{1}{\mu} \delta(\mu - \mu') \Sigma$$

the transport equation for  $\mu > 0$  is

$$\frac{\partial}{\partial x} \phi(x, \mu) = \int_0^1 B(\mu, \mu') \phi(x, \mu') d\mu' \quad (4.45)$$

and for the albedo problem the initial condition which specifies  $\phi(0, \mu)$  will be known.

We note in passing that equation (4.45) admits of a solution in series, obtained by integrating once to read

$$\phi(x, \mu) = \phi(0, \mu) + \int_0^x dt \int_0^1 B(\mu, \mu') \phi(t, \mu') d\mu'$$

and then using successive substitutions to give

$$\begin{aligned} \phi(x, \mu) = \phi(0, \mu) + \sum_{i=1}^I \frac{x^i}{i!} \int_0^1 B^{(i)}(\mu, \mu') \phi(0, \mu') d\mu' \\ + R_I. \end{aligned} \quad (4.46)$$

The remainder term  $R_I$  is given by

$$R_I = \frac{1}{I!} \int_0^x (x-t)^I dt \int_0^1 B^{(I+1)}(\mu, \mu') \phi(t, \mu') d\mu'$$

and the matrices  $B^{(i)}(\mu, \mu')$  are defined recursively by

$$\begin{aligned} B^{(1)}(\mu, \mu') &\equiv B(\mu, \mu') \\ B^{(i+1)}(\mu, \mu') &= \int_0^1 B(\mu, \mu'') B^{(i)}(\mu'', \mu') d\mu'' \quad i \geq 1. \end{aligned}$$

Provided  $x$  is sufficiently small the remainder term in equation (4.46) will tend to zero with increasing  $I$  so that the series expansion implicit in equation (4.46) will converge and produce the required solution. Goldstein and Brooks (1963) have pointed out in a different context that series obtained by this repeated substitution method are essentially Neumann series solutions and

will converge rapidly for small enough  $x$ . It is to be noted that if the matrices  $B^{(i)}(\mu, \mu')$  remain bounded as  $i \rightarrow \infty$  then the series will converge for all  $x$ , like the exponential series for  $e^x$  which has an obvious similarity to the series solution.

For a numerical solution of the albedo problem in a discrete ordinate approximation we begin by writing equation (4.45) in the form

$$\frac{\partial}{\partial x} \phi(x, \mu_i) = \sum_{j=1}^M \omega_j B(\mu_i, \mu_j) \phi(x, \mu_j)$$

where the discrete ordinates  $\mu_i$ ,  $i = 1, 2, \dots, M$  lie in the range  $0 < \mu \leq 1$ , and  $\omega_i$  are the corresponding quadrature weights for integration with respect to  $\mu$  over this range. A series solution corresponding to that in equation (4.46) can now be developed for the  $\phi(x, \mu_i)$  vector, but like the exponential series this is useless for numerical work when  $x$  is large. Instead we construct a vector  $\psi(x)$  with  $NM$  elements

$$\begin{aligned} \psi_1(x) &= \phi_1(x, \mu_1) \\ \psi_2(x) &= \phi_1(x, \mu_2) \\ &\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ \psi_M(x) &= \phi_1(x, \mu_M) \\ \psi_{M+1}(x) &= \phi_2(x, \mu_1) \\ &\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ &\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ \psi_{NM}(x) &= \phi_N(x, \mu_M) \end{aligned}$$

and write the revised form of equation (4.45) as

$$\frac{d}{dx} \underset{\sim}{\psi}(x) = \underset{\sim}{B} \underset{\sim}{\psi}(x). \quad (4.47)$$

The matrix  $\underset{\sim}{B}$  has the block form

$$\underset{\sim}{B} = \begin{pmatrix} (D^{11}) & (D^{12}) & \dots & (D^{1N}) \\ (\underset{\sim}{D}^{21}) & (\underset{\sim}{D}^{22}) & & (\underset{\sim}{D}^{2N}) \\ (\underset{\sim}{D}^{N1}) & (\underset{\sim}{D}^{N2}) & & (\underset{\sim}{D}^{NN}) \end{pmatrix}$$

where the matrices  $(\underset{\sim}{D}^{ij})$  have components

$$(\underset{\sim}{D}^{ij})_{k\ell} = \omega_{\ell} B_{ij}(\mu_k, \mu_{\ell}).$$

The matrix differential equation (4.47) is a well known problem and its solution by classical methods is discussed by Goertzel and Tralli (1960), who write the solution as

$$\underset{\sim}{\psi}(x) = e^{\underset{\sim}{x}\underset{\sim}{B}} \underset{\sim}{\psi}(0). \quad (4.48)$$

Their treatment depends on evaluation of all eigenvectors and eigenvalues of the matrix  $\underset{\sim}{B}$  which is then diagonalised to give

$$\underset{\sim}{B} = \underset{\sim}{S} \underset{\sim}{\Lambda} \underset{\sim}{S}^{-1}$$

in the usual notation,  $\underset{\sim}{\Lambda}$  being the diagonal matrix whose diagonal elements are the various eigenvalues  $\lambda_i$  of  $\underset{\sim}{B}$ . The

matrix exponential is then simply

$$e^{\tilde{X}\tilde{B}} = \tilde{S} e^{\tilde{X}\tilde{\Lambda}} \tilde{S}^{-1}$$

and  $e^{\tilde{X}\tilde{\Lambda}}$  is a diagonal matrix with diagonal elements  $e^{\tilde{X}\lambda_1}$ ,  $e^{\tilde{X}\lambda_2}$ , etc. Aesthetically pleasing though such a treatment may be it suffers from at least two disadvantages when applied to large scale problems. Firstly storage is required for both  $\tilde{S}$ , the matrix of eigen columns, and its inverse  $\tilde{S}^{-1}$ . Secondly a really fast and foolproof routine for finding all eigenvalues and eigenvectors of an arbitrary large matrix has yet to be developed, the claims of numerical analysts and scientific subroutine package writers notwithstanding.

The need for solutions to large sets of equations like (4.47) arises in connection with the analysis of pulsed neutron experiments (e.g. Maher, Ritchie and Rainbow 1968) and in this context the truncated power series expansion method of Barnard et al (1963) is commonly used. This method expresses the matrix exponential as

$$e^{\tilde{X}\tilde{B}} \approx \left\{ \tilde{I} + \frac{\tilde{X}}{n} \tilde{B} \left( \tilde{I} + \frac{1}{2} \left( \frac{\tilde{X}}{n} \right) \tilde{B} \left( \tilde{I} + \frac{1}{3} \left( \frac{\tilde{X}}{n} \right) \tilde{B} \left( \tilde{I} + \frac{1}{4} \left( \frac{\tilde{X}}{n} \right) \tilde{B} \right) \right) \right) \right\}^n$$

where  $n$  is chosen sufficiently large to ensure that the absolutely large eigenvalue of the matrix  $\frac{\tilde{X}}{n} \tilde{B}$  is sufficiently smaller than unity and therefore that truncation of the power series after



five terms supplies adequate accuracy. Although fast and foolproof this method still requires that three times the storage necessary for  $\underline{\mathcal{B}}$  be reserved; once for  $\underline{\mathcal{B}}$  itself, once for terms like  $\left(\underline{\mathcal{I}} + \frac{1}{4} \frac{\underline{x}}{\underline{n}} \underline{\mathcal{B}}\right)$  and once for their product.

In our work we chose to use a procedure which minimised storage requirements but sacrificed some speed. The procedure used the Pade approximant for  $e^t$

$$e^t \approx \frac{1 + \frac{1}{2}t}{1 - \frac{1}{2}t}$$

in the corresponding matrix form

$$\begin{aligned} e^{\underline{A}} &\approx (\underline{\mathcal{I}} + \frac{1}{2} \underline{A}) (\underline{\mathcal{I}} - \frac{1}{2} \underline{A})^{-1} \\ &= 4(2\underline{\mathcal{I}} - \underline{A})^{-1} - \underline{\mathcal{I}}. \end{aligned}$$

Writing

$$\underline{A} = 2^{-n} \times \underline{\mathcal{B}}$$

it follows that

$$e^{\underline{A}} \approx \left\{ \left( \frac{1}{2} \underline{\mathcal{I}} - 2^{-(n+2)} \times \underline{\mathcal{B}} \right)^{-1} - \underline{\mathcal{I}} \right\}^{2n} \quad (4.49)$$

$$= \underline{Q}^{2n} \quad (\text{say})$$

and the error can be made as small as desired by choosing  $n$  large enough. For arbitrary matrices  $\underline{\mathcal{B}}$  the storage requirements for this procedure are simply twice that necessary to store  $\underline{\mathcal{B}}$  itself. After  $\underline{\mathcal{B}}$  is computed its elements can be overwritten by the elements of  $\frac{1}{2} \underline{\mathcal{I}} - 2^{-(n+2)} \times \underline{\mathcal{B}}$ . The successive operations of matrix inversion and subtraction of the identity matrix need

no additional storage and produce the matrix  $\tilde{Q}$ . The successive squarings to give the sequence  $\tilde{Q}^2, \tilde{Q}^4, \tilde{Q}^8, \dots, \tilde{Q}^n$  can then be performed in just twice the storage necessary to contain  $\tilde{Q}$  itself.

Not even this penalty has to be paid for the important application to slowing down problems discussed in Section 4.6 since the matrix  $\tilde{B}$  is then block lower triangular with all blocks  $(\tilde{D}^{ij})$  being null when  $i < j$ . Clearly in a computer programme, storage need not be allocated to these null matrices and this almost halves the storage requirements for  $\tilde{B}$  (and for  $\tilde{Q}$  which also is lower triangular). The successive squarings for  $\tilde{Q}$  can also be performed if additional storage is allocated for two blocks each the size of the  $\tilde{D}^{ij}$  matrices.

The appropriate algorithms to use for matrices  $\tilde{Q}$  which are block lower triangular of the form

$$\tilde{Q} = \begin{pmatrix} \tilde{Q}^{11} & 0 & 0 & 0 \\ \tilde{Q}^{21} & \tilde{Q}^{22} & 0 & 0 \\ \tilde{Q}^{31} & \tilde{Q}^{32} & \tilde{Q}^{33} & 0 \\ \tilde{Q}^{N1} & \tilde{Q}^{N2} & \tilde{Q}^{N3} & \tilde{Q}^{NN} \end{pmatrix}$$

are:

(a) to invert  $\tilde{Q}$

(i) (set  $\tilde{Q}^{ii} = (\tilde{Q}^{ii})^{-1}$ ), for  $i = 1, 2, \dots, N$ , and then

(ii) ((set  $\tilde{Q}^{ij} = -\tilde{Q}^{ii} \sum_{\ell=j}^{i-1} \tilde{Q}^{i\ell} \tilde{Q}^{\ell j}$ ), for  $j = 1, 2, \dots, i-1$ ),  
for  $i = 2, 3, \dots, N$ ,

and (b) to square  $\tilde{Q}$

$$\left( \left( \text{set } \tilde{Q}^{ij} = \sum_{\ell=j}^i \tilde{Q}^{i\ell} \tilde{Q}^{\ell j} \right), \text{ for } j = 1, 2, \dots, i \right),$$

for  $i = N, N-1, \dots, 2, 1$ .

With the matrix  $e^{\tilde{x}\tilde{B}}$  evaluated from equation (4.49) repeated application of equation (4.48) gives successively  $\tilde{\psi}(x)$ ,  $\tilde{\psi}(2x)$ ,  $\tilde{\psi}(3x)$ , ... so that the forward going angular fluxes can easily be evaluated at a regular mesh of space points in the medium. With the forward going angular fluxes evaluated the backward going angular fluxes can be found by application of equations (4.2) written in the form

$$\tilde{\phi}(x, -\mu_i) = \frac{1}{2\mu_i} \sum_j \omega_j \tilde{S}(\mu_i, \mu_j) \tilde{\phi}(x, +\mu_j) \quad (4.50)$$

whilst the group scalar fluxes can be evaluated by noting that equation (4.10a) is only a special case of the more general result

$$\tilde{\phi}(x) = \int_0^1 \tilde{V}^0(\mu) \tilde{\phi}(x, +\mu) d\mu \quad (4.51)$$

which is written for numerical purposes as

$$\tilde{\phi}(x) = \sum_j \omega_j \tilde{V}^0(\mu_j) \tilde{\phi}(x, \mu_j).$$

#### 4.7.1 Numerical Solution of the Adjoint Albedo Problem

We now describe briefly the numerical methods necessary for solution of the adjoint albedo problem. Here the adjoint

transport equation (4.13) has to be solved subject to the boundary conditions that  $\phi^*(0, -\mu)$  is a known vector function and that  $\phi^*(x, \mu)$  is bounded as  $x \rightarrow \infty$ .

The analysis is in every way similar to that just followed for the regular transport equation and only the essential points will be given. After using equations (4.8) and (4.11), the adjoint equation is written

$$\Sigma \phi^*(x, -\mu) + \mu \frac{\partial}{\partial x} \phi^*(x, -\mu) = \frac{1}{2} \sum_{\ell} P_{\ell}(-\mu) \tilde{C}_{\ell}^{\ell} \int_0^1 \tilde{U}^{\ell}(\mu') \phi^*(x, -\mu') d\mu'$$

with

$$\phi^*(x, \mu) = \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \phi^*(x, -\mu') d\mu' \quad (4.52)$$

or simply

$$\frac{\partial}{\partial x} \phi^*(x, -\mu) = \int_0^1 B^*(\mu, \mu') \phi^*(x, -\mu') d\mu' \quad (4.53)$$

where

$$B^*(\mu, \mu') = \frac{1}{2\mu} \sum_{\ell} P_{\ell}(-\mu) \tilde{C}_{\ell}^{\ell} \tilde{U}^{\ell}(\mu') - \frac{1}{\mu} \delta(\mu - \mu') \Sigma.$$

Since equation (4.53) is essentially similar to equation (4.45) the same technique can be applied to solve it and the angular adjoints  $\phi^*(x, -\mu)$  can be evaluated in the discrete directions  $\mu_i$ . Equation (4.52) in the discrete ordinate form determines the angular adjoints  $\phi^*(x, -\mu)$ . The scalar adjoints are determined from the equation

$$\phi^*(x) = \int_0^1 \tilde{U}^0(\mu) \phi^*(x, -\mu) d\mu$$

which is the adjoint equivalent of equation (4.51).

Both regular and adjoint albedo problems can then be solved by this numerical technique.

#### 4.8 Solutions for Two Semi Infinite Media

Throughout the present chapter we have been concerned with establishing a method for finding solutions (both analytic and numerical) of the multigroup transport equation in a semi infinite slab. The motivation for the study (if one is needed) lies in the fact that the semi infinite medium solutions will be used in the following chapter to find approximate solutions to a class of realistic transport problems in finite but thick slabs. Before proceeding, however, it is instructive to consider a physically realistic problem to which the semi infinite medium analysis has immediate application. The configuration for the problem is two different semi infinite media meeting at the plane  $x = 0$  with a uniform source of particles on that plane. The physical problem we have in mind is the "shielding bench-mark problem" of C.W. Garret as reported by Profio (1969) where the two semi infinite media are the air and the ground, while the source at the air/ground interface is the gamma ray source  $\text{Co}_{60}$  supposed distributed uniformly over the ground. The problem as posed is to calculate, amongst other quantities, the

gamma dose and the gamma ray number flux density at a point three feet above the ground. Although the problem is one of gamma ray transport rather than neutron transport the multigroup approximation can still be used for energy dependence and a transport equation of the same form as equation (4.1) will still be appropriate in each of the two half spaces.

The equations to be solved are therefore

$$\Sigma_1 \phi(x, \mu) + \mu \frac{\partial}{\partial x} \phi(x, \mu) = \frac{1}{2} \sum_{\ell} P_{\ell}(\mu) C_1^{\ell} \int_{-1}^1 P_{\ell}(\mu') \phi(x, \mu') d\mu' \quad 0 < x < \infty$$

$$-1 < \mu < 1$$
(4.54)

$$\Sigma_2 \phi(x, \mu) + \mu \frac{\partial}{\partial x} \phi(x, \mu) = \frac{1}{2} \sum_{\ell} P_{\ell}(\mu) C_2^{\ell} \int_{-1}^1 P_{\ell}(\mu') \phi(x, \mu') d\mu' \quad -\infty < x < 0$$

$$-1 < \mu < 1$$
(4.55)

where the suffices 1 and 2 refer to the materials in the left and right hand half spaces respectively. The source conditions at the interface  $x = 0$  are represented by the equations

$$\left. \begin{aligned} \phi(0+, +\mu) &= \phi(0-, +\mu) + \frac{1}{\mu} q(+\mu) \\ \phi(0-, -\mu) &= \phi(0+, -\mu) + \frac{1}{\mu} q(-\mu) \end{aligned} \right\} \quad 0 < \mu \leq 1 \quad (4.56)$$

where  $\phi(0+, +\mu) = \lim_{x \rightarrow 0+} \phi(x, +\mu)$  etc.

In equations (4.56) the vector  $q(\mu)$  in an  $N$  group problem has

elements

$$q_1(\mu), q_2(\mu) \dots q_i(\mu) q_N(\mu)$$

where  $q_i(\mu)d\mu$  is the number of particles released by the source in group  $i$  per square cm. per sec. whose direction cosines lie in the range  $\mu$  to  $\mu + d\mu$ .

If solutions are sought in region 2, the half space where  $x$  is positive, these can be obtained by the methods developed in the previous section provided that the angular fluxes entering the half space can be evaluated, for then the problem is essentially the albedo problem for this half space.

To this end we calculate for the two materials reflection matrices denoted by  $\tilde{S}_1(\mu, \mu')$  and  $\tilde{S}_2(\mu, \mu')$ , evaluating them in terms of matrices  $\tilde{U}_1^\ell(\mu)$ ,  $\tilde{V}_1^\ell(\mu)$ ,  $\tilde{U}_2^\ell(\mu)$  and  $\tilde{V}_2^\ell(\mu)$  in accordance with the analysis of earlier sections. In terms of these matrices the following relationships will hold between angular fluxes in the neighbourhood of the interface

$$\left. \begin{aligned} \tilde{\phi}(0+, -\mu) &= \frac{1}{2\mu} \int_0^1 \tilde{S}_2(\mu, \mu') \tilde{\phi}(0+, +\mu') d\mu' \\ \tilde{\phi}(0-, +\mu) &= \frac{1}{2\mu} \int_0^1 \tilde{S}_1(\mu, \mu') \tilde{\phi}(0-, -\mu') d\mu' \end{aligned} \right\} \quad (4.57)$$

After eliminating all angular fluxes but  $\phi(0+, +\mu)$  between equations (4.56), (4.57) it follows that

$$\begin{aligned}
2\mu \phi(0+, +\mu) - \int_0^1 \left\{ \int_0^1 \tilde{S}_1(\mu, \mu'') \tilde{S}_2(\mu'', \mu') \frac{d\mu''}{2\mu''} \right\} \phi(0+, +\mu') d\mu' \\
= 2\tilde{q}(\mu) + \int_0^1 \frac{\tilde{S}_1(\mu, \mu') \tilde{q}(-\mu')}{\mu'} d\mu'.
\end{aligned} \tag{4.58}$$

If as in Garrett's benchmark problem the source is an isotropic one in each group then

$$\tilde{q}(\mu) = \frac{1}{2} \tilde{Q}$$

where the elements of the vector  $\tilde{Q}$  are the source strengths in the various groups, equation (4.58) becomes simply

$$\begin{aligned}
2\mu \phi(0+, +\mu) - \int_0^1 \left\{ \int_0^1 \tilde{S}_1(\mu, \mu'') \tilde{S}_2(\mu'', \mu') \frac{d\mu''}{2\mu''} \right\} \phi(0+, +\mu') d\mu' \\
= \tilde{U}_1^0(\mu) \tilde{Q}.
\end{aligned} \tag{4.59}$$

For numerical work a discrete ordinate representation for all angular variations is appropriate and then equations (4.58) or (4.59) become simply a set of inhomogeneous linear equations for the vectors  $\phi(0+, +\mu_j)$  which can be solved by standard techniques. The marching procedure described in section (4.7) can then be used to generate the solution at any required point in the right hand half space.

The candidate has not carried out the solution procedure for the air/ground benchmark problem because no suitable gamma ray data were available at the time this thesis



was written. When data are available it is proposed to rectify this situation.

## 5. MULTIGROUP THEORY FOR A FINITE SLAB

We are now in a position to study the multigroup transport problem which prompted this whole dissertation - the multigroup transport problem in a finite slab with a neutron source impinging on one face. For many such problems a detailed knowledge of the group fluxes in the interior of the slab is not wanted and the quantity of interest will be some functional of the group angular fluxes emerging from one or other face of the slab. The example which comes immediately to mind is that of estimating the neutron dose transmitted through a slab  $0 \leq x \leq a$  when a given angular neutron source impinges on the face at  $x = 0$ . The quantity of interest would then, in the notation of chapter 4, be

$$\mathcal{L} = \int_0^1 \mu \tilde{D} \tilde{\phi}(a, \mu) d\mu$$

where the row vector  $\tilde{D}$  contained as elements the current to dose conversion factors in the various groups. For some other problem however  $\mathcal{L}$  could be a weighted sum of currents reflected back from the slab face  $x = 0$ .

For a homogeneous slab, solutions of such problems may be tackled by extending to the multigroup situation the concept of the X- and Y- functions which were studied in chapter 3, and such a treatment is conceptually feasible if

the various group to group transfer reactions are assumed isotropic in the laboratory system. However such a treatment has to contend with the difficulty of tabulating the functions for all possible transfer matrices. If to this is added the complexities introduced into the analysis by the fact that the group to group transfers are far from isotropic, it becomes clear that an alternative method is necessary. As well as avoiding these difficulties the method to be proposed will deal with slabs which are only piecewise homogeneous and the method can thus be used for study of laminated shields.

### 5.1 Statement of the Problem

We suppose the slab to lie between  $x = x_0 \equiv 0$  and  $x = x_N \equiv a$  and to consist of  $N$  homogeneous layers with interfaces at points  $x_1, x_2, \dots, x_{N-1}$ . In each of these layers the transport equation appropriate to the material of the layer is to be satisfied and across the interfaces the angular fluxes are to be continuous. The source conditions imposed are that the vector  $\underline{\phi}(x, \mu)$  of group angular fluxes is known at  $x = 0$  for  $0 < \mu \leq 1$  and is zero at the free boundary  $x = a$  for  $-1 \leq \mu < 0$ . Thus specifically it is required that for  $n = 1, 2, \dots, N$

$$\Sigma \underline{\phi}(x, \mu) + \mu \frac{\partial \underline{\phi}(x, \mu)}{\partial x} = \frac{1}{2} \sum_{\ell} C_{\ell}^{\ell} P_{\ell}(\mu) \int_{-1}^1 P_{\ell}(\mu') \underline{\phi}(x, \mu') d\mu', \quad -1 \leq \mu \leq 1 \quad (5.1)$$

$$x_{n-1} \leq x \leq x_n,$$

$$\text{that } \underline{\phi}(x_0, \mu) = \underline{\phi}_0(\mu) \text{ the given source distribution, } 0 < \mu \leq 1, \quad (5.2)$$

$$\underline{\phi}(x_N, \mu) = 0 \quad -1 \leq \mu < 0 \quad (5.3)$$

and for  $n = 1, 2, \dots, N-1$  that

$$\phi(x_n^+, \mu) - \phi(x_n^-, \mu) = 0 \quad -1 < \mu < 1 \quad (5.4)$$

The integral of interest will be taken as

$$I = \int_0^1 \mu \tilde{T}(\mu) \phi(x_N, \mu) d\mu - \int_0^1 \mu \tilde{R}(\mu) \phi(x_0, \mu) d\mu \quad (5.5)$$

where the column vectors  $\tilde{T}(\mu)$  and  $\tilde{R}(\mu)$  are appropriate weighting functions for transmitted and reflected group angular fluxes. Either  $\tilde{T}(\mu)$  or  $\tilde{R}(\mu)$  can of course be zero vectors for particular problems.

## 5.2 The Variational Formula

The method consists in estimating the integral  $I$  by means of a variational principle and is thus an extension of the method used in chapter 3 for estimating the  $X$ - and  $Y$ -functions of Chandrasekhar.

The variational formula is constructed according to the procedure described by Lewins (1965a, 1965b). We replace the functions  $\phi(x, \mu)$  by a trial function  $\psi(x, \mu)$ , which should be subject to the constraints imposed by equations (5.1 - 5.4), multiply each constraint by an undetermined multiplier and integrate them over the range of interest of the problem. This resulting integral added to the integral of interest in (5.5) becomes the functional to be studied. From the requirement that the first variation of the functional be zero with respect to

changes in the trial function  $\psi(x, \mu)$  a number of equations sufficient to fix the undetermined multipliers can then be found.

The appropriate functional is

$$\begin{aligned}
 \mathcal{L} = & \int_0^1 \mu \tilde{T}(\mu) \tilde{\psi}(x_N, \mu) d\mu - \int_{-1}^0 \mu \tilde{R}(\mu) \tilde{\psi}(x_0, \mu) d\mu \\
 & + \sum_{n=1}^N \int_{x_{n-1}}^{x_n} dx \int_{-1}^1 d\mu \tilde{\psi}^*(x, \mu) \left\{ \frac{1}{2} \sum_{\ell} C_{\ell}^{\ell} P_{\ell}(\mu) \int_{-1}^1 P_{\ell}(\mu') \tilde{\psi}(x, \mu') d\mu' \right. \\
 & \quad \left. - \sum \tilde{\psi}(x, \mu) - \mu \frac{\partial}{\partial x} \tilde{\psi}(x, \mu) \right\} \\
 & + \int_{-1}^0 \mu \tilde{\psi}^*(x_N, \mu) \tilde{\psi}(x_N, \mu) d\mu - \int_0^1 \mu \tilde{\psi}^*(x_0, \mu) \left\{ \tilde{\psi}(x_0, \mu) - \tilde{\phi}_0(\mu) \right\} d\mu \\
 & - \sum_{n=1}^{N-1} \int_0^1 \mu \tilde{\psi}^*(x_n, \mu) \left\{ \tilde{\psi}(x_n, \mu) - \tilde{\psi}(x_n, \mu) \right\} d\mu \\
 & - \sum_{n=1}^{N-1} \int_{-1}^0 \mu \tilde{\psi}^*(x_n, \mu) \left\{ \tilde{\psi}(x_n, \mu) - \tilde{\psi}(x_n, \mu) \right\} d\mu
 \end{aligned} \tag{5.6}$$

in which the  $\tilde{\psi}^*(x, \mu)$  are the undetermined multipliers. If in the multiple integral term of equation (5.6), the order of the  $\mu$  and  $\mu'$  integrations is reversed and a partial  $x$ -integration is carried out, the functional may be written in the alternative form

$$\begin{aligned}
\mathcal{L} = & \int_0^1 \mu \tilde{\psi}(x_N, \mu) \left\{ T(\mu) - \tilde{\psi}^*(x_N, \mu) \right\} d\mu - \int_{-1}^0 \mu \tilde{\psi}(x_0, \mu) \left\{ R(\mu) - \tilde{\psi}^*(x_0, \mu) \right\} d\mu \\
& + \sum_{n=1}^N \int_{x_{n-1}}^{x_n} dx \int_{-1}^1 \tilde{\psi}(x, \mu) \left\{ \frac{1}{2} \sum_{\ell} \tilde{C}_{\ell}^{\ell} P_{\ell}(\mu) \int_{-1}^1 P_{\ell}(\mu') \tilde{\psi}^*(x, \mu') d\mu' - \sum_{\ell} \tilde{\psi}^*(x, \mu) + \mu \frac{\partial}{\partial x} \tilde{\psi}^*(x, \mu) \right\} d\mu \\
& + \int_0^1 \mu \tilde{\psi}^*(x_0, \mu) \phi_0(\mu) d\mu \\
& + \sum_{n=1}^{N-1} \int_0^1 \mu \tilde{\psi}(x_n, \mu) \left\{ \tilde{\psi}^*(x_n, \mu) - \tilde{\psi}^*(x_n, -\mu) \right\} d\mu \\
& + \sum_{n=1}^{N-1} \int_{-1}^0 \mu \tilde{\psi}(x_n, \mu) \left\{ \tilde{\psi}^*(x_n, \mu) - \tilde{\psi}^*(x_n, -\mu) \right\} d\mu. \tag{5.7}
\end{aligned}$$

From the form (5.7) it is easy to see that the first variation of  $\mathcal{L}$  with respect to the trial function  $\tilde{\psi}(x, \mu)$  is zero provided that  $\tilde{\psi}^*(x, \mu)$  is the solution to the adjoint equation (4.13) in each of the layers  $x_{n-1} \leq x \leq x_n$ , that the angular adjoints are continuous across each of the interfaces and that  $\tilde{\psi}^*(x, \mu)$  satisfies the boundary conditions

$$\begin{aligned}
\tilde{\psi}^*(x_0, \mu) &= R(\mu) & -1 \leq \mu < 0 \\
\tilde{\psi}^*(x_N, \mu) &= T(\mu) & 0 < \mu \leq 1.
\end{aligned}$$

In addition, from (5.6), it can be seen that  $\mathcal{L}$  is stationary with respect to changes in  $\tilde{\psi}^*(x, \mu)$  if the trial function  $\tilde{\psi}(x, \mu)$  is the solution to the problem posed by

equations (5.1 - 5.4) and the stationary value of  $\mathcal{L}$  is simply  $I$ , the integral of interest.

To estimate  $I$  we evaluate the functional  $\mathcal{L}$  using as reasonable a set of trial functions  $\psi(x, \mu)$  and  $\psi^*(x, \mu)$  as can be constructed.

### 5.3 Generation of Trial Functions

As trial functions it is reasonable to select the solutions of appropriately chosen semi infinite medium problems (both regular and adjoint types). Thus in the first layer  $x_0 < x < x_1$ ,  $\psi(x, \mu)$  is chosen as the solution of the albedo problem for a medium identical with that of the layer and with incident angular fluxes given by

$$\psi(x_0, \mu) = \phi_0(\mu), \quad 0 < \mu \leq 1.$$

This trial function, which can be computed to any desired degree of precision by the methods described in the previous chapter, need only be evaluated at the end points  $x_0$  and  $x_1$  of the layer and there give the trial function values

$$\psi(x_0, \mu), \quad \psi(x_1, \mu), \quad -1 \leq \mu \leq 1.$$

Because this trial function  $\psi(x, \mu)$  satisfies the transport equation (5.1) throughout the layer, its contribution to the multiple integral term in equation (5.6) is identically zero. The forward going angular fluxes  $\psi(x_1, \mu)$ ,  $\mu > 0$  are continued

across the interface  $x_1$  to give suitable initial values  $\psi(x_1+, \mu)$  for the angular fluxes in the next layer. A semi infinite medium solution can then be generated for the material of this second layer and will provide the trial function values  $\tilde{\psi}(x_1+, \mu), \mu < 0$  and  $\tilde{\psi}(x_2-, \mu), -1 \leq \mu \leq 1$ . Again the actual values of the trial function  $\tilde{\psi}(x, \mu)$  in the interior of this layer are not required since their contribution to the multiple integral term in equation (5.1) will be identically zero. This process can be repeated for each layer in turn until finally the trial values  $\tilde{\psi}(x_N, \mu)$  are obtained and the complete trial function has been generated.

Because the trial function  $\tilde{\psi}(x, \mu)$  has been selected to satisfy the appropriate transport equation in each layer, to satisfy the initial condition (5.2), and to be continuous across the interfaces when  $\mu > 0$ , the functional  $\mathcal{L}$  to be evaluated becomes simply

$$\begin{aligned} \mathcal{L} = & \int_0^1 \mu \tilde{T}(\mu) \tilde{\psi}(x_N, \mu) d\mu - \int_{-1}^0 \mu \tilde{R}(\mu) \tilde{\psi}(x_0, \mu) d\mu \\ & + \int_{-1}^0 \mu \tilde{\psi}^*(x_N, \mu) \tilde{\psi}(x_N, \mu) d\mu \\ & - \sum_{n=1}^{N-1} \int_{-1}^0 \mu \tilde{\psi}^*(x_n, \mu) \left\{ \tilde{\psi}(x_n+, \mu) - \tilde{\psi}(x_n-, \mu) \right\} d\mu. \end{aligned} \quad (5.8)$$



The construction of an adjoint trial function  $\psi^*(x, \mu)$  is done in three parts. First an adjoint trial function  $\psi_R^*(x, \mu)$  is constructed which approximates the solution of the adjoint problem for which  $T(\mu) \equiv 0$ . Then a trial function  $\psi_T^*(x, \mu)$  is constructed to approximate the solution of the  $R(\mu) = 0$  problem, and finally these two approximations are added together. This addition is justifiable on the grounds that the adjoint equation is linear. Of course only one step has to be carried out if it is solely the transmitted neutrons which are of interest and this is the case for deep penetration problems in reactor shields. Identical methods would be used for generation of the trial function  $\psi_R^*(x, \mu)$  so that only the method adopted for generation of  $\psi_T^*(x, \mu)$  will here be described. The boundary conditions for  $\psi_T^*(x, \mu)$  are

$$\psi_T^*(x_N, \mu) = T(\mu) \quad \mu > 0$$

$$\psi_T^*(x_0, \mu) = 0 \quad \mu < 0$$

The procedure used is similar to that used for generating the trial function  $\psi(x, \mu)$  in that it uses semi infinite medium solutions within each layer in turn. Starting with the layer  $x_{N-1} \leq x \leq x_N$  the solution is generated to the semi infinite medium adjoint problem appropriate to the region  $-\infty < x \leq x_N$ , with material properties identical to the last layer

and with boundary conditions  $\tilde{\psi}^*(x_N, \mu) = T(\mu)$ ,  $\mu > 0$ . This solution is continued in the negative  $x$  direction until the interface  $x = x_{N-1}$  is reached and gives, for  $-1 < \mu < 1$ , trial values of  $\tilde{\psi}^*(x_N, \mu)$  and of  $\tilde{\psi}^*(x_{N-1}^+, \mu)$ . The angular adjoints with  $\mu > 0$  are then continued across the interface to give  $\tilde{\psi}^*(x_{N-1}^-, \mu)$ ,  $\mu > 0$  and these used as boundary conditions for a semi infinite medium adjoint problem in the region  $-\infty < x \leq x_{N-1}$ , using the material properties of the layer  $x_{N-2} \leq x \leq x_{N-1}$ . The solution of this semi infinite problem then supplies, for  $-1 \leq \mu \leq 1$ , the trial values needed of  $\tilde{\psi}^*(x_{N-1}^-, \mu)$  and  $\tilde{\psi}^*(x_{N-2}^+, \mu)$ . This layer by layer procedure is followed until the first layer has been treated and all trial values needed for  $\tilde{\psi}_T^*(x, \mu)$  have been found. Clearly this trial function will not satisfy the requirement of continuity across the interfaces with  $\mu < 0$ , though the construction procedure produces continuity for  $\mu > 0$ , and it is tempting to try to generate some better trial function. We have resisted this temptation since it would always be present, unless an exact solution of the adjoint problem had been constructed throughout the slab, and in that case we may as well have solved the original transport problem instead.

The generation of the trial function  $\tilde{\psi}_R^*(x, \mu)$  is performed in a similar way except that it is started at the first slab with  $\tilde{\psi}_R^*(x_0, \mu) = R(\mu)$ ,  $\mu < 0$  and the angular adjoints

$\psi_R^*(x_n^+, \mu)$  are made continuous for  $\mu < 0$ .

#### 5.4 Description of Test Problems

In chapter 3 it was found that the equivalent one group procedure produced more accurate integrals for the reflected angular fluxes than for those transmitted and it is likely that the corresponding result will be true for the present multigroup theory. In testing the accuracy of the method therefore we have restricted ourselves to estimating integrals of transmitted angular fluxes in a number of test situations, three of which are now described.

In the first test problem (Problem A) neutron transmissions were required through a single homogeneous slab of a nominal Australian concrete. The slab thickness was 120 cm. and the concrete (of density  $2.08 \text{ gm cm}^{-3}$ ) was treated in nine energy groups of lethargy width 0.25 starting from lethargy 0.0 (energy 10 MeV.) and finishing at lethargy 2.25 (energy 1.0 MeV.). The anisotropy of the group to group scattering reactions was treated by a  $P_3$  approximation, while those scattering reactions which would transfer neutrons to energies below that of the ninth energy group were treated as absorptions. Microscopic cross sections for the concrete constituents were taken from the UKAEA nuclear data file (Norton, 1968) and were group averaged by conventional methods

over an integrated fission spectrum.

The source condition chosen was that of an isotropic plane source in group 1, the highest energy group, of a strength sufficient to produce an incoming current of  $10^6 \text{ n.cm.}^{-2} \text{ sec}^{-1}$  and the integral of interest was the current transmitted through the slab in group 9.

In studying this problem the aim was to find out the effect (on the computed value of the integral of interest) of inaccuracies in computing the  $\tilde{U}^\ell(\mu), \tilde{V}^\ell(\mu)$  matrix elements from the equations (4.11a), (4.12a).

Problem B was identical with problem A except that the thickness of the concrete slab was varied in the range from 10 cm. to 200 cm. From experience with one group problems studied in Chapter 3 it was expected that use of the variational method would be most satisfactory for slabs of large thickness and the aim in this study was to see how large a "large" slab should be.

For problem C the slab consisted of nine alternating layers of iron and water, with of course an iron layer at each end. The thicknesses of the various layers starting from the source plane were 1 inch, 1 inch, 2 inches, 2 inches, 3 inches, 2 inches, 3 inches, 13 inches, and 9 inches, making a total thickness of 3 feet. This arrangement was part of a neutron shield design proposed, at one stage, for the U.K.A.E.A. Steam

Generating Heavy Water Reactor (Greenhalgh et.al., 1967).

The source condition chosen in each energy group was an isotropic plane source of strength sufficient to produce an incoming neutron current of  $6.318 \times 10^{10} \text{ n.cm.}^{-2} \text{ sec}^{-1}$  in the nine groups combined. This incoming current was distributed between the nine groups in proportion to the fission spectrum. The quantity of interest was the total neutron current transmitted through the slab in the nine groups. The treatment of cross sections, for this problem, was the same as that for Problem A, that is  $P_3$  scattering with all cross section data taken from the UKAEA Nuclear Data File.

In studying this problem the main aim was to find out how effective the variational method proposed in sections (5.2), (5.3) would be in allowing for discontinuities in material properties. A subsidiary aim was to find out in general terms how accurately the trial fluxes for a discontinuous problem could approximate the true scalar fluxes in a realistic problem.

### 5.5 Computer Codes

To perform calculations for the test problems a FORTRAN programme was written embodying the techniques described in this chapter and the preceding one. The calculations were carried out on the IBM 360/50 computer at the Australian Atomic

Energy Commission's Research Establishment. Since upscattering was not present in any of the test problems, the programme, in calculating the  $\tilde{U}^{\ell}(\mu), \tilde{V}^{\ell}(\mu)$  matrices, used the solution strategy described in Section (4.6). Iterations were continued until the proportional change in the individual matrix elements during an iteration was below some prescribed tolerance or else until some maximum number of iterations had been exceeded. Angular integrations over the ranges  $0 < \mu < 1$  or  $-1 < \mu < 0$  were performed by the Radau quadrature scheme so that angular fluxes in the directions  $\mu = \pm 1$  were calculated explicitly. Once calculated, the  $\tilde{U}^{\ell}(\mu), \tilde{V}^{\ell}(\mu)$  matrices for a particular material were stored on a magnetic disk so that they could be used in any later problems which involved that material. As well as these matrices the elements of the corresponding reflection matrix  $\tilde{S}(\mu, \mu')$  were also saved against later need.

As part of the problem specification it was decided that the programme user should specify, for each homogeneous region in the slab, not only the material number for the region but the number and size of mesh intervals for the region. As necessary the programme is then able to calculate, for each size mesh interval, the elements of the corresponding transmission matrix  $e^{\tilde{X}\tilde{B}}$  defined in equations (4.48), (4.49) and these too are saved on magnetic disk for use in other regions or in other problems. In the programme, the transmission matrix

is used to generate the trial fluxes at each successive mesh point where they are printed out, but of course they need only be calculated at region boundaries to estimate transmissions through the full slab. In a typical problem, the generation of the transmission matrices takes a significant fraction of the total computing time for the problem and the technique of storing the transmission matrix to avoid recomputing it for use in some other region gives worthwhile savings in total computing time. Against this saving has to be traded off the penalty of input-output time required for the disk transfers but no attempt was made to save this time beyond buffering the information in blocks of 1600 bytes.

All calculations were performed in double precision arithmetic (64 bits).

For all the test problems the "correct" solutions were assumed to be those found by the discrete ordinate code SLABBO (Clancy, 1969b), which solved the transport problems by the iterative methods described in chapter 1.

## 5.6 Results for Test Problem Calculations

### 5.6.1 Problem A

All calculations for this problem were performed using an  $S_8$  approximation for the angular fluxes.

The "exact" solution used 60 equally spaced mesh intervals of 2 cm. each, took 4.8 minutes computing time and gave, for the group 9 transmitted current, a value of  $2.9963 \text{ n. cm}^{-2} \cdot \text{sec}^{-1}$ .

Using the procedures evolved in the present work the answers obtained are given in Table 5.1.

Variational Method Solutions for Problem A

Group 9 Current $\text{n. cm}^{-2} \cdot \text{sec}^{-1}$ .	Computing Time mins.	Accuracy of Computed $\tilde{U}^{\ell}(\mu)\tilde{V}^{\ell}(\mu)$ Matrices
2.5894	3.2	only 1 iteration allowed
2.9448	3.2	only 2 iterations allowed
2.9887	3.3	only 3 iterations allowed
2.9894	3.5	change $<10^{-2}$ on last iteration
2.9943	3.5	change $<10^{-3}$ on last iteration
2.9949	3.5	change $<10^{-4}$ on last iteration
2.9949	3.5	change $<10^{-5}$ on last iteration

TABLE 5.1

From these results we have extracted a rule of thumb that the accuracy to which the  $\tilde{U}^{\ell}(\mu)\tilde{V}^{\ell}(\mu)$  matrices are computed is about the same as the accuracy of the final answer.

The case where only one iteration was allowed was selected to give a guide to the possibility of using the first iterate of equations (4.11a), (4.12a) to give us an approximation



to the matrix  $\underline{U}^\ell(\mu)$ ,

$$\begin{aligned} U_{mn}^\ell(\mu) = & P_k(-\mu) \delta_{mn} \\ & + \frac{\mu}{2} \sum_{\ell} (-)^{\ell} P_{\ell}(-\mu) C_{mn}^{\ell} \int_0^1 \frac{P_k(\mu') P_{\ell}(-\mu')}{\mu \sigma_n + \mu' \sigma_m} d\mu' \end{aligned}$$

with a similar approximation for  $\underline{V}^\ell(\mu)$ , since an attempt to evaluate the integral analytically would then be worthwhile. The results for problem A show that this first iterate is not very satisfactory, but they also show that iteration to high accuracy is not very expensive in terms of computing time. For the remaining test problems an accuracy of  $10^{-6}$  in the  $\underline{U}^\ell(\mu), \underline{V}^\ell(\mu)$  matrices was routinely demanded.

#### 5.6.2 Problem B

For these calculations an  $S_8$  approximation was again used. For the "exact" solutions equally spaced mesh intervals of 2.0 cm. were used throughout but for the variational method mesh intervals of 10.0 cm were used, with the result that the regular and adjoint transmission matrices then only had to be calculated once for solution of all the problems.

The results obtained are shown in Table 5.2

Solutions for Problem B

Concrete Thickness cm.	Exact Solutions		Variational Solutions	
	Gp.9 Current $\text{n.cm}^{-2}.\text{sec}^{-1}$ .	Computing Time mins.	Gp.9 Current $\text{n.cm}^{-2}.\text{sec}^{-1}$ .	Computing Time mins.
10	$1.2341 \cdot 10^{-2}$	0.98	$1.2068 \cdot 10^{-2}$	3.75
20	$6.8211 \cdot 10^{-3}$	1.75	$6.7943 \cdot 10^{-3}$	.87
40	$1.5436 \cdot 10^{-3}$	1.90	$1.5416 \cdot 10^{-3}$	.87
80	$7.0710 \cdot 10^{-5}$	3.61	$7.0661 \cdot 10^{-5}$	.90
120	$2.9963 \cdot 10^{-6}$	4.83	$2.9950 \cdot 10^{-6}$	.92
160	$1.2129 \cdot 10^{-7}$	7.12	$1.2125 \cdot 10^{-7}$	.95
200	$4.7791 \cdot 10^{-9}$	8.85	$4.7779 \cdot 10^{-9}$	.97

TABLE 5.2

The trend in the results is quite as expected. The error in the variational solutions decreases with increasing thickness of slab, which reflects the fact that the semi infinite medium trial fluxes are better approximations to the real fluxes when the slab gets thicker. The computing times indicate the considerable saving achieved by storing the transmission matrices computed for the case of the 10. cm slab.

The errors themselves are all acceptable when the thickness is at least 20 cm, which is about 5 mean free paths.

5.6.3 Problem C

These calculations were performed using an  $S_{12}$  approximation for the angular fluxes, earlier calculations having

shown that this was adequate to predict the transmitted current to better than 0.1 percent accuracy.

For the exact calculation mesh intervals of 0.5 ins were used in the iron regions and 0.2 ins in the water. Computing time was 15.0 minutes and the total transmitted current was found to be  $24578 \text{ n.cm}^{-2}.\text{sec}^{-1}$ .

The variational calculation was made initially using mesh intervals of 1 inch in both materials, which the code subdivided internally of course. This calculation took 16.3 mins. and the estimate for the total current was  $24463. \text{ n.cm}^{-2}.\text{sec}^{-1}$ . which is in error by .47%.

The variational calculation was then repeated using the same set of mesh intervals as in the "exact" calculation so as to have a set of group trial fluxes suitable for comparison with those of the exact calculation.

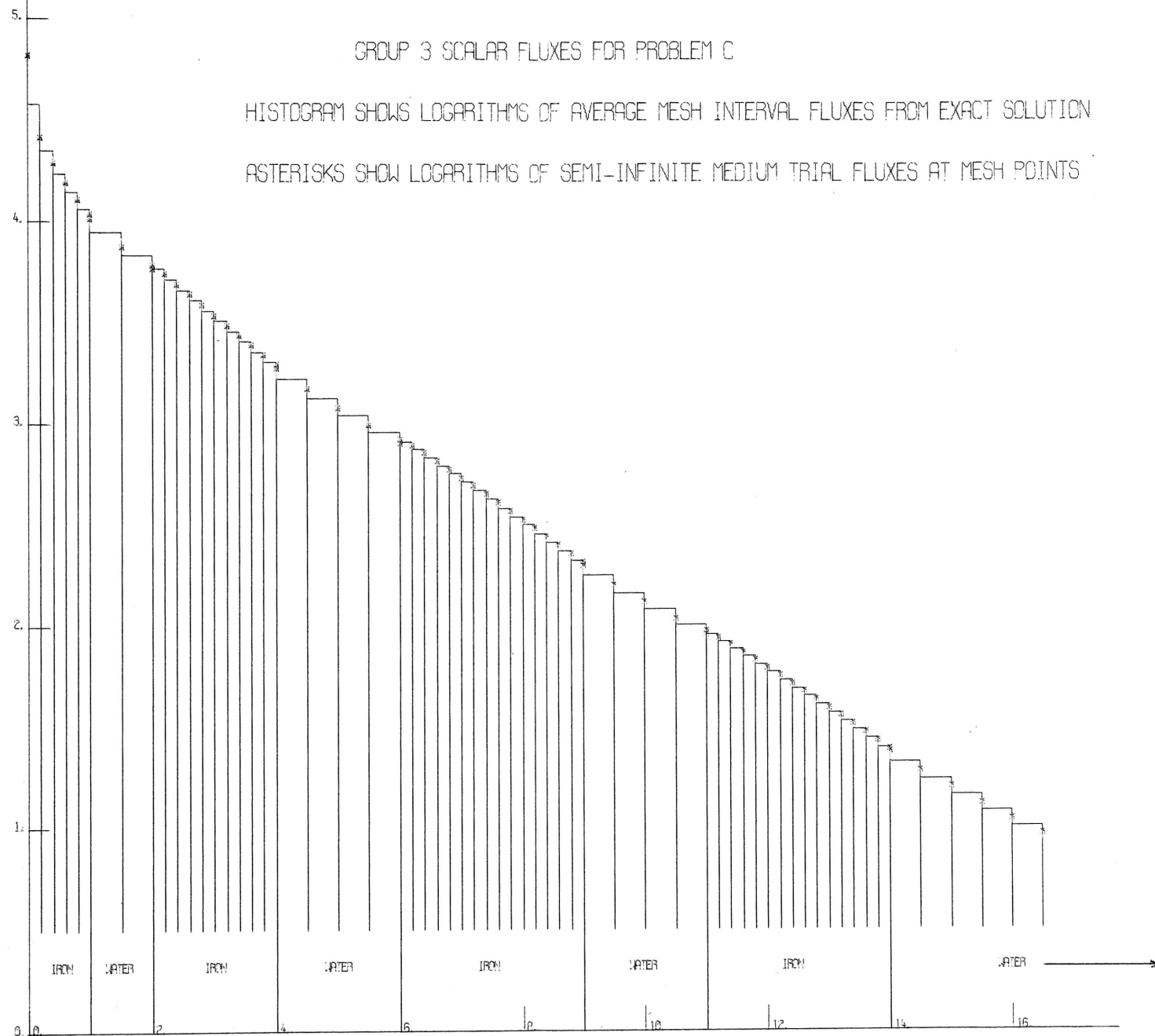
Figure 5.1 shows the two sets of fluxes in group 3 - selected for no very good reason, but typical of the behaviour of the other groups. The histogram-like entries on this graph are the average flux in the mesh intervals calculated by the "exact" calculation, the points marked \* are the trial function fluxes which are discontinuous at the material boundaries. The overall agreement in group 3 - as in the other groups - is very

FIGURE 5.1

GROUP 3 SCALAR FLUXES FOR PROBLEM C

HISTOGRAM SHOWS LOGARITHMS OF AVERAGE MESH INTERVAL FLUXES FROM EXACT SOLUTION

ASTERISKS SHOW LOGARITHMS OF SEMI-INFINITE MEDIUM TRIAL FLUXES AT MESH POINTS



good except near material interfaces and near the free boundary remote from the source, though this latter defect does not show in Figure 5.1.

### 5.7 Utility of the Method

Though the results of the test problems do not bring this out, the variational method has the drawback that the time required for a significant part of the calculation will depend roughly on the second or third power of  $NG/2$ , where  $N$  is the  $S_N$  order and  $G$  is the number of groups. This time penalty, which is masked in many problems by time spent in other calculations and in performing input output, is incurred by the need to compute the transmission matrices for a mesh interval and to use them in calculating the angular fluxes at each successive mesh point. All other things being equal this time penalty can be reduced by selecting an optimum number of mesh intervals for a region.

Doubling the number of mesh intervals in a region reduces by one the number of squarings of the partial transmission matrix  $Q$  which have to be made to derive the final matrix from that calculated according to equation (4.49). For each squaring the number of arithmetic operations is proportional to  $(NG)^3$ , and to transmit the angular fluxes across a mesh interval the number is proportional to  $6(NG)^2$ . A little elementary analysis

then shows that the optimum number of mesh intervals for a single region is  $(NG/4)$ .

Even with this optimisation the time for the evaluation of the transmission matrix for a given region is still dependent on at least the square of  $NG$ . For a single many group problem this is probably too much of a penalty to pay and the calculation is better performed by direct methods. For a set of calculations made on the same system, but varying the source condition, or on a number of systems with various region thicknesses, the facility for storing transmission matrices once computed can make the variational method an attractive proposition.

The accuracy of the estimated integrals of the transmitted fluxes is good for very large homogeneous slabs and is reasonable for thick slabs consisting of a number of quite thin regions such as the system in Problem C. The accuracy could certainly be improved if a better estimate of adjoint function could be obtained but for the reasons pointed out near the end of Section 5.3 we have to be content with the present method, which should be retained for those situations where its advantages can be utilised.

## 6. FURTHER APPLICATIONS OF THE REFLECTION FUNCTION METHOD

In earlier chapters it has been our concern to show the applicability of the reflection function technique to neutron transport problems in one dimensional plane geometry where information is sought about angular fluxes of the form  $\phi(x, \mu)$ . Such problems do not, however, exhaust the range of application of the reflection function concept and in this chapter we shall describe briefly the application of the method to a number of other transport problems. All of these will be discussed using one group theory for simplicity but all of them will permit generalisation to a multigroup treatment.

### 6.1 Inhomogeneous Semi Infinite Media

We consider a medium occupying the half space  $0 \leq x < \infty$ , with absorption and scattering cross sections being functions of  $x$  alone. If position in the medium is measured in units of total mean free paths from the boundary  $x = 0$ , the one dimensional source free transport equation for an isotropically scattering medium can be written

$$\phi(z, \mu) + \mu \frac{\partial \phi}{\partial z} = \frac{c(z)}{2} \int_{-1}^1 \phi(z, \mu') d\mu' \quad (6.1)$$

where  $\frac{dz}{dx} = \sigma(x)$  the total cross section at position  $x$  and  $c(z)$  is the ratio of scattering to total cross section at position  $x$ .

If we now impose suitable boundary conditions on the flux at the boundary  $z = x = 0$  and on its limiting value as  $z \rightarrow \infty$  the transport problem is completely posed.

Proceeding as in Chapter 2 it is possible to separate the angular fluxes into forward and backward going components  $\phi(z, +\mu)$ ,  $\phi(z, -\mu)$  and to relate them for  $\mu > 0$  by the equation

$$\phi(z, -\mu) = \frac{1}{2\mu} \int_0^1 S(z, \mu, \mu') \phi(z, \mu') d\mu' \quad (6.2)$$

where the reflection function  $S$  now depends explicitly on  $z$ .

An equation can be derived for  $S(z, \mu, \mu')$  exactly as in the homogeneous medium problem by choosing an initial condition

$$\phi(0, +\mu) = \delta(\mu - \mu_0) \quad 0 < \mu, \mu_0 \leq 1$$

and then determining the spatial derivative of the angular fluxes at  $z = 0$  in terms of the reflection function  $S(z, \mu, \mu')$ . Inserting these expressions into the derivative of equation (6.2) leads to the equation

$$\begin{aligned} \left( \frac{1}{\mu} + \frac{1}{\mu_0} \right) S(z, \mu, \mu_0) - \frac{\partial}{\partial z} S(z, \mu, \mu_0) \\ = c(z) H(z, \mu) H(z, \mu_0) \end{aligned} \quad (6.3)$$

$$\text{where } H(z, \mu) = 1 + \int_0^1 \frac{S(z, \mu, \mu')}{2\mu'} d\mu' \quad (6.4)$$

$$\text{or} \quad = 1 + \int_0^1 \frac{S(z, \mu', \mu)}{2\mu'} d\mu' .$$



These equations have been discussed by Bellman and Kalaba (1965).

## 6.2 Problems with Azimuthal Variation

In all applications considered so far the direction of neutron travel has only been characterised by  $\mu$ , the cosine of the angle between the neutron direction and the normal to the medium boundary (usually  $x = 0$ ) and the azimuthal variation of angular flux has been ignored.

If the material scatters isotropically then the angular flux after a collision has no azimuthal variation but in situations involving anisotropically scattering materials, the azimuthal variation will be present and can be important. As an example of such a situation we quote the problem of calculating neutron transmissions through ducts in thick shields. A standard method for making the calculation is described by Selph and Claiborne (1968), who use a Monte Carlo treatment for the neutron paths through the duct and allow the neutrons to be reflected from the concrete walls of the duct in accordance with the double differential albedo calculation of Maercker and Muckenthaler (1965). These double differential albedos, themselves calculated by Monte Carlo methods, describe the probability that a neutron will be reflected from a semi infinite medium in specified directions. We shall show how the reflection function treatment may be used to calculate this double differential

albedo directly.

Allowing for azimuthal variation the source free neutron transport equation for a homogeneous semi infinite medium  $0 \leq x < \infty$  may be written with  $\mu > 0$  as

$$\phi(x, \pm\mu, \theta) \pm \mu \frac{\partial}{\partial x} \phi(x, \pm\mu, \theta) = \int_{-1}^1 d\mu' \int_0^{2\pi} d\theta' \sigma(\mu' \theta' \rightarrow \mu \theta) \phi(x, \mu', \theta') \quad (6.5)$$

where the position coordinate  $x$  is measured in units of mean free path and  $\cos^{-1} \mu$ ,  $\theta$  are the spherical polar angles describing the neutron direction  $\underline{\Omega}$ . The differential scattering cross section  $\sigma(\mu' \theta' \rightarrow \mu \theta)$  may be expanded in terms of its Legendre polynomial components  $\sigma^\ell$  as

$$\begin{aligned} \sigma(\mu' \theta' \rightarrow \mu \theta) &= \frac{1}{4\pi} \sum_{\ell} \sigma^\ell P_{\ell}(\underline{\Omega} \cdot \underline{\Omega}') \\ &= \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \sum_{k=-\ell}^{\ell} a_{\ell k} P_{\ell}^k(\mu') \cos k(\theta - \theta'), \end{aligned} \quad (6.6)$$

where  $a_{\ell k} = \sigma^\ell (\ell - |k|)! / (\ell + |k|)!$

and  $P_{\ell}^k(\mu)$  are the associated Legendre functions,

so that  $P_{\ell}^{-k}(\mu) = P_{\ell}^k(\mu)$

and  $P_{\ell}^0(\mu) \equiv P_{\ell}(\mu)$ .

The forward and backward going angular fluxes  $\phi(x, +\mu, \theta)$ ,  $\phi(x, -\mu, \theta)$  are then related by the reflection function  $S(\mu, \theta; \mu' \theta')$  according to the equation

$$\phi(x, -\mu, \theta) = \frac{1}{2\mu} \int_0^1 d\mu' \int_0^{2\pi} d\theta' S(\mu, \theta; \mu', \theta') \phi(x, +\mu', \theta') \quad (6.7)$$

to the right hand side of which can be added a term  $\phi_X(x, -\mu, \theta)$  if any neutrons are born in the interior of the semi infinite medium.

Clearly if it is possible to determine the reflection function then the double differential albedo for the medium can be found.

If the incoming flux has azimuthal symmetry

$$\phi(x, +\mu, \theta) = \frac{1}{2\pi} \phi(x, +\mu)$$

then the outgoing flux  $\phi(x, -\mu, \theta)$  will have the same symmetry

so that 
$$\phi(x, -\mu, \theta) = \frac{1}{2\pi} \phi(x, -\mu)$$

and in terms of the ordinary reflection function of Chapter 2

$$\phi(x, -\mu) = \frac{1}{2\mu} \int_0^1 S(\mu, \mu') \phi(x, +\mu') d\mu'.$$

Substituting those results into equation (6.7) it follows

that 
$$\int_0^{2\pi} S(\mu, \theta; \mu', \theta') d\theta' = S(\mu, \mu'). \quad (6.8)$$

To obtain an equation for the reflection function  $S(\mu, \theta; \mu', \theta')$  the now well established procedure is followed. The incident angular flux at the boundary  $x = 0$  is chosen as

$$\phi(0, +\mu, \theta) = \delta(\mu - \mu_0) \delta(\theta - \theta_0), \quad 0 < \mu, \mu_0 \leq 1$$

$$0 < \theta, \theta_0 \leq 2\pi$$

so that the emerging angular distribution is

$$\phi(0, -\mu, \theta) = \frac{1}{2\mu} S(\mu, \theta; \mu_o, \theta_o).$$

Using equation (6.5) the spatial derivatives of the angular fluxes on the boundary are then expressed in terms of the reflection function. After differentiating equation (6.7) with respect to  $x$  and setting  $x = 0$  these spatial derivatives can then be eliminated and the resulting equation is

$$\begin{aligned} \frac{1}{2} \left( \frac{1}{\mu} + \frac{1}{\mu_o} \right) S(\mu, \theta; \mu_o, \theta_o) &= \sigma(\mu_o, \theta_o \rightarrow -\mu, \theta) \\ &+ \int_0^1 \frac{d\mu'}{2\mu'} \int_0^{2\pi} d\theta' \sigma(\mu_o, \theta_o \rightarrow \mu', \theta') S(\mu, \theta; \mu', \theta') \\ &+ \int_0^1 \frac{d\mu''}{2\mu''} \int_0^{2\pi} d\theta'' \sigma(-\mu'', \theta'' \rightarrow -\mu, \theta) S(\mu_o, \theta_o; \mu'', \theta'') \\ &+ \int_0^1 \frac{d\mu'}{2\mu'} \int_0^{2\pi} d\theta' \int_0^1 \frac{d\mu''}{2\mu''} \int_0^{2\pi} d\theta'' S(\mu_o, \theta_o; \mu'', \theta'') \sigma(-\mu'', \theta'' \rightarrow \mu', \theta') S(\mu, \theta; \mu', \theta'). \end{aligned}$$

If the expression (6.6) for the scattering cross section is used the equation for the reflection function may be written after some manipulation as

$$\begin{aligned} &\left( \frac{1}{\mu} + \frac{1}{\mu_o} \right) S(\mu, \theta; \mu_o, \theta_o) \\ &= \frac{1}{2\pi} \sum_{\ell} \sum_{k=-\ell}^{\ell} (-)^{\ell} a_{\ell k} \left\{ \phi_{\ell}^k(\mu, \theta) \phi_{\ell}^k(\mu_o, \theta_o) + \psi_{\ell}^k(\mu, \theta) \psi_{\ell}^k(\mu_o, \theta_o) \right\} \quad (6.9) \end{aligned}$$

where

$$\phi_{\ell}^k(\mu, \theta) = P_{\ell}^k(-\mu) \cos k\theta + \int_0^1 \frac{d\mu'}{2\mu'} \int_0^{2\pi} d\theta' P_{\ell}^k(\mu') \cos k\theta' S(\mu, \theta; \mu', \theta') \quad (6.10)$$

$$\psi_{\ell}^k(\mu, \theta) = P_{\ell}^k(-\mu) \sin k\theta + \int_0^1 \frac{d\mu'}{2\mu'} \int_0^{2\pi} d\theta' P_{\ell}^k(\mu') \sin k\theta' S(\mu, \theta; \mu', \theta') \quad (6.11)$$

For  $k = 0$  it follows that

$$\psi_{\ell}^0(\mu, \theta) = 0$$

and

$$\phi_{\ell}^0(\mu, \theta) = P_{\ell}(-\mu) + \int_0^1 \frac{d\mu'}{2\mu'} P_{\ell}(\mu') \int_0^{2\pi} S(\mu, \theta; \mu', \theta') d\theta'.$$

Equation (6.8) implies that

$$\phi_{\ell}^0(\mu, \theta) = P_{\ell}(-\mu) + \int_0^1 \frac{d\mu'}{2\mu'} P_{\ell}(\mu') S(\mu, \mu')$$

and from equation (2.35) it follows that

$$\phi_{\ell}^0(\mu, \theta) = \phi_{\ell}(\mu), \text{ the Busbridge } \phi \text{ function.}$$

From equations (6.10) and (6.11) it is clear that

$$\phi_{\ell}^{-k}(\mu, \theta) = \phi_{\ell}^k(\mu, \theta)$$

and

$$\psi_{\ell}^{-k}(\mu, \theta) = -\psi_{\ell}^k(\mu, \theta)$$

so that only the functions with  $k$  positive have to be determined from equations (6.9) - (6.11). To determine these functions equation (6.9) is substituted into (6.10) and (6.11) giving

$$\begin{aligned}
\phi_{\ell}^k(\mu, \theta) &= P_{\ell}^k(-\mu) \cos k\theta \\
&+ \frac{\mu}{4\pi} \sum_m \sum_{n=-m}^m (-)^m a_{mn} \phi_m^n(\mu, \theta) \int_0^1 \frac{d\mu'}{\mu+\mu'} P_{\ell}^k(\mu') \int_0^{2\pi} d\theta' \cos k\theta' \phi_m^n(\mu', \theta') \\
&+ \frac{\mu}{4\pi} \sum_m \sum_{n=-m}^m (-)^m a_{mn} \psi_m^n(\mu, \theta) \int_0^1 \frac{d\mu'}{\mu+\mu'} P_{\ell}^k(\mu') \int_0^{2\pi} d\theta' \cos k\theta' \psi_m^n(\mu', \theta')
\end{aligned} \tag{6.12}$$

with an equation for  $\psi_{\ell}^k(\mu, \theta)$  differing only in the replacement of the terms  $\cos k\theta$  and  $\cos k\theta'$  by  $\sin k\theta$  and  $\sin k\theta'$  respectively. Like the equations (2.36) for the  $\phi_{\ell}(\mu)$  functions, these equations can be solved iteratively and from their solutions and equation (6.9) the reflection function  $S(\mu, \theta; \mu_0, \theta_0)$  can be reconstructed.

### 6.3 Time Dependent Problems

In this application we shall consider one group neutron transport in a homogeneous semi infinite medium which we take to have isotropic scattering. Distance  $x$  from the boundary plane  $x = 0$  and time  $t$  are measured in units for which the total cross section and the neutron speed are both unity. The transport equation in the absence of volume sources is then

$$\phi(x, \mu, t) + \frac{\partial \phi}{\partial t} + \mu \frac{\partial \phi}{\partial x} = \frac{c}{2} \int_{-1}^1 \phi(x, \mu', t) d\mu' \tag{6.13}$$

for which typically, solutions would be sought subject to the boundary conditions

$$\left. \begin{aligned} \phi(x, \mu, t) &= 0 & t < 0 \\ \lim_{x \rightarrow \infty} \phi(x, \mu, t) &= 0 & t > 0 \\ \phi(0, \mu, t) &= f(\mu, t) & \mu > 0, t \geq 0 \end{aligned} \right\} \quad (6.14)$$

= a defined source function.

A reflection function  $S(\mu, \mu', t')$  can then be defined which relates the incoming and outgoing angular fluxes by the equation

$$\phi(x, -\mu, t) = \frac{1}{2\mu} \int_0^1 d\mu' \int_0^\infty dt' \phi(x, \mu', t-t') S(\mu, \mu', t') \quad (6.15)$$

so that  $t'$  corresponds to the time elapsing between particles passing the  $x$  plane in directions  $+\mu'$  and being reflected back through that plane in directions  $-\mu$ . From physical arguments it is clear that

$$S(\mu, \mu', t') = 0 \quad \text{if } t' < 0. \quad (6.16)$$

To evaluate  $S$  the boundary conditions are taken to be those given in equations (6.14)

with  $f(\mu, t) = \delta(\mu - \mu_0) \delta(t)$ .

Equation (6.15) then is at  $x = 0$

$$\phi(0, -\mu, t) = \frac{1}{2\mu} \int_0^1 d\mu' \int_0^t dt' \phi(0, \mu', t-t') S(\mu, \mu', t')$$

so that

$$\phi(0, -\mu, t) = \frac{1}{2\mu} S(\mu, \mu_0, t) \quad \mu, t > 0$$

and 
$$\frac{\partial \phi}{\partial t}(0, -\mu, t) = \frac{1}{2\mu} \frac{\partial S}{\partial t}(\mu, \mu_0, t) \quad \mu, t > 0$$

whilst 
$$\phi(0, \mu, t) = \delta(\mu - \mu_0) \delta(t) \quad \mu, t \geq 0$$

$$\frac{\partial \phi}{\partial t}(0, \mu, t) = \delta(\mu - \mu_0) \delta'(t) \quad \mu, t \geq 0.$$

From here on the procedure follows the usual path.

The transport equation (6.13) is used to evaluate at  $x = 0$  the spatial derivatives of the angular fluxes in terms of the reflection function and these forms inserted into the result of differentiating equation (6.15) with respect to  $x$  and then setting  $x = 0$ . The equation which results from this analysis is

$$\begin{aligned} & \frac{1}{c} \left( \frac{1}{\mu} + \frac{1}{\mu_0} \right) \{ S(\mu, \mu_0, t) + \frac{\partial}{\partial t} S(\mu, \mu_0, t) \} \\ &= \delta(t) + \int_0^1 \frac{d\mu'}{2\mu'} S(\mu, \mu', t) + \int_0^1 \frac{d\mu''}{2\mu''} S(\mu'', \mu_0, t) \\ &+ \int_0^t dt' \int_0^1 \frac{d\mu'}{2\mu'} \int_0^1 \frac{d\mu''}{2\mu''} S(\mu, \mu', t') S(\mu'', \mu_0, t-t') \end{aligned}$$

With  $H(\mu, t) = \delta(t) + \int_0^1 \frac{d\mu'}{2\mu'} S(\mu, \mu', t)$  (6.17)



it follows that

$$\left(\frac{1}{\mu} + \frac{1}{\mu_0}\right) \left(1 + \frac{\partial}{\partial t}\right) S(\mu, \mu_0, t) = c \int_0^t dt' H(\mu_0, t') H(\mu, t-t').$$

With the initial condition (6.16) this can be solved as a differential equation to give

$$S(\mu, \mu_0, t) = \frac{c\mu\mu_0}{\mu+\mu_0} \int_0^t dt' e^{-(t-t')} \int_0^{t'} dt'' H(\mu_0, t'') H(\mu, t'-t'') \quad (6.18)$$

and so give for the H function an equation

$$H(\mu, t) = \delta(t) + \frac{c\mu}{2} \int_0^t \frac{d\mu'}{\mu+\mu'} \int_0^t dt' e^{-(t-t')} \int_0^{t'} dt'' H(\mu', t'') H(\mu, t'-t''). \quad (6.19)$$

From the starting condition

$$\lim_{t \rightarrow 0+} [H(\mu, t) - \delta(t)] = 0$$

this equation for  $H(\mu, t)$  can be solved numerically and then the reflection function  $S(\mu, \mu', t)$  can be found from equation (6.18).

It is interesting to note that when the Laplace Transform of equation (6.19) is taken with respect to the time variable the resulting equation is

$$\bar{H}(\mu, p) = 1 + \frac{c}{1+p} \frac{\mu}{2} \bar{H}(\mu, p) \int_0^1 \frac{H(\mu', p)}{\mu+\mu'} d\mu'$$

which is of course the equation for the time independent H-function for a medium with the average number of secondary neutrons per collision equal to  $c/(1+p)$ , which is complex.

#### 6.4 A Final Remark

Clearly it would be possible to describe a number of other problems to which the reflection function techniques could be applied - with more or less success. We believe it has been demonstrated that the method is most useful for those problems in which the only information wanted about the solution of the transport equation is its behaviour on the material boundaries or else when approximate solutions in the interior of the medium may themselves be used to generate corrected approximations on the boundaries e.g. by a variational technique. We do not claim that the method should replace the conventional methods for solution of transport problems, but rather that the method can have a place in the already large armoury of solution techniques and should be used when it is appropriate.

# REFERENCES

- ABRAMOWITZ, M., & STEGUN I.A., (1965), "Handbook of Mathematical Functions", Dover Publications Inc., New York. N.Y.
- AMBARZUMIAN V.A., (1942), Astron.J.Soviet Union, 19, 30.
- AMBARZUMIAN V.A., (1943), Compt.rend.Acad.Sci. URSS, 38, 229.
- AUERBACH T., (1961), Report BNL 676.
- BARNARD E., KHAN N.A., MCLATCHIE R.C.F., POOLE M.J. & TAIT J.H., (1963) Nucl.Sci.& Engng., 17, 513.
- BELLMAN R., & KALABA R., (1965), "Quasilinearization and Nonlinear Boundary-Value Problems", American Elsevier Publishing Company, Inc., New York, N.Y.
- BELLMAN R., KALABA R. & PRESTRUD M., (1962), "Invariant Imbedding and Radiative Transfer in Slabs of Finite Thickness", The Rand Corporation.
- BELLMAN R., KALABA R. & WING G.M., (1960), J.Math.Phys., 1, 40.
- BUSBRIDGE I.W., (1960), "The Mathematics of Radiative Transfer", Cambridge University Press, England.
- CARLSON B., (1953), Report LA 1599.
- CARLSON B. & BELL G.I., (1958), Proc.Second Intern.Conf.Peaceful Uses of Atomic Energy, 16, 535.
- CASE K.M., (1960), Ann.Phys. (N.Y.), 9, 1.
- CASE K.M., DE HOFFMAN F. & PLACZEK G., (1953), "Introduction to the Theory of Neutron Diffusion, Vol. 1.", US Govt. Printing Office.

- CASE K.M. & ZWEIFEL P.F., (1967), "Linear Transport Theory",  
Addison-Wesley, Reading.Mass.
- CHANDRASEKHAR S., (1944), Astrophys.J., 100, 76.
- CHANDRASEKHAR S., (1948), Astrophys.J., 108, 92.
- CHANDRASEKHAR S., (1949), Astrophys.J., 109, 555.
- CHANDRASEKHAR S., (1960), "Radiative Transfer", Dover Publications  
Inc., New York, N.Y.
- CHANDRASEKHAR S., ELBERT D. & FRANKLIN A., (1952), Astrophys.J.,  
115, 244.
- CLANCY B.E., (1969a), Aust.J. Phys., 22, 317.
- CLANCY B.E., (1969b), Report AAEC-TM505.
- CLANCY B.E., (1970), J.nucl.Energy, (in press), also report AAEC-TM 529.
- CLANCY B.E. & DONNELLY I.J., (1970), Nucl.Sci.& Engng., 39, 398.
- CLIFFORD C.E., MYNATT F.R. & STRAKER E.A., (1969), Nuclear News,  
12, 2, 51.
- DAVISON B., (1957), "Neutron Transport Theory", Clarendon Press,  
Oxford. England.
- ENGLE W.W.Jr., (1967), Report K1963.
- ENGLE W.W.Jr. & MYNATT F.R., (1968), Trans.Am.Nucl.Soc., 11, 193.
- GLASSTONE S. & EDLUND M.C., (1952), "The Elements of Nuclear Reactor  
Theory", Van Nostrand Co.Inc., Princeton, N.J.
- GOERTZEL G. & TRALLI N., (1960), "Some Mathematical Methods of  
Physics", McGraw Hill Book Co. New York, N.Y.
- GOLDSTEIN R. & BROOKS H., (1963), Nucl.Sci. & Engng., 17, 534.
- GREEN C., (1967), Report AEEW-R498.

- GREENHALGH F.G., PAGET F.T.W., SMITH D.R. & TRUELOVE J.P., (1967),  
Proc. London Symposium Engng. Aspects of the Winfrith  
S.G.H.W.R.
- HORAK H.G., (1952), Astrophys.J., 110, 477.
- LEONARD A. & FERZIGER J.H., (1966), Nucl.Sci. & Engng. 26, 181.
- LEWINS J., (1965a), "Importance - The Adjoint Function",  
Pergamon Press Ltd., Oxford, England.
- LEWINS J., (1965b), Unpublished seminar delivered to Yaphank  
Philosophical Society.
- MAERKER R.E., & MUCKENTHALER F.J., (1965), Nucl.Sci. & Engng.,  
22, 455.
- MAHER K.J., RITCHIE A.I.M. & RAINBOW M.T., (1968), Conference  
on Neutron Thermalization & Reactor Spectra, IAEA, Vienna.
- MAYERS D.F., (1962), Mon.Not.R.astr.Soc., 123, 483.
- MULLIKIN T.W., (1962), Astrophys.J., 136, 627.
- MULLIKIN T.W., (1964), "Non linear Integral Equations", ed.P.M.Anselone,  
Univ. of Wisconsin Press, Madison, Wisc.
- MYNATT F.R., MUCKENTHALER F.J. & STEVENS P.N., (1969),  
Report CTC-INF-952.
- NOBLE B., (1964), "Nonlinear Integral Equations", ed.P.M.Anselone,  
Univ. of Wisconsin Press, Madison, Wis.
- PAHOR S., (1966), Nucl.Sci. & Engng., 26, 192.
- PAHOR S., (1967), Nucl.Sci. & Engng., 29, 248.

- PAHOR S., (1968), Nucl.Sci. & Engng. 31, 110.
- PAHOR S. & SHULTIS J.K., (1969a), J.nucl.Energy, 23, 477.
- PAHOR S. & SHULTIS J.K., (1969b), J.Math.Phys., 10, 2220.
- PAHOR S. & ZWEIFEL P.F., (1969), J.Math.Phys., 10, 581.
- PROFIO A.E., (1969), Report ORNL-RSIC-25.
- RYSHIK I.M. & GRADSTEIN I.S., (1963), "Tables of Series, Products and Integrals", VEB Deutscher Verlagder Wissenschaften, Berlin.
- SELPH W.E. & CLAIBORNE H.C., (1968), Report ORNL-RSIC-20.
- SELPH W.E., (1968), Report ORNL-RSIC-21.
- SHULTIS J.K., (1969), Nucl.Sci.& Engng., 38, 83.
- SHURE F. & NATELSON M., (1964), Ann.Phys., 26, 274.
- SIEWERT C.E. & SHIEH P.S., (1967), J.nucl.Energy, 21, 383.
- SIEWERT C.E. & ZWEIFEL P.F., (1966), J.Math.Phys., 7, 2092.
- SOBOLEV V.V., (1963), "A Treatise on Radiative Transfer",  
D. van Nostrand Inc., Princeton, N.J.
- SPENCER L.V., DIAZ J.A. & MOSES E., (1964), Report NBS-8542.
- VAN DE HULST H.C., (1948), Astrophys.J., 107, 220.
- WHITTAKER E.T & WATSON G.N., (1927), "A Course of Modern  
Analysis", Cambridge University Press, England.
- WICK G.C., (1943), Z. Phys., 121, 702.
- YOSHIMURA T. & KATSURAGI S., (1968), Nucl.Sci. & Engng, 33, 297.
- ZELAZNY R. & KUSZELL A., (1961), Ann.Phys., (N.Y.), 16, 81.

APPENDIXPROPERTIES OF THE MATRICES  $U^\ell(\mu)$  AND  $V^\ell(\mu)$ A.1 The Legendre Moments of  $U^\ell(\mu)$  and  $V^\ell(\mu)$ 

We derive in this section a number of relationships between the Legendre moments, defined as matrices

$$\tilde{M}^{qk} = \int_0^1 P_q(\mu) \tilde{U}^\ell(\mu) d\mu$$

$$\tilde{N}^{qk} = \int_0^1 P_q(\mu) \tilde{V}^\ell(\mu) d\mu.$$

If equation (4.11a) is multiplied by  $\sigma_n P_q(\mu)$  it may be written after use of the relation

$$\frac{\mu \sigma_n}{\mu \sigma_n + \mu' \sigma_m} = 1 - \frac{\mu' \sigma_m}{\mu \sigma_n + \mu' \sigma_m}$$

as

$$\begin{aligned} \sigma_n P_q(\mu) U_{mn}^k(\mu) &= \sigma_n \delta_{mn} P_q(\mu) P_k(-\mu) \\ &+ \frac{1}{2} \sum_{\ell} (-)^\ell \sum_{ij} P_q(\mu) U_{mi}^\ell(\mu) C_{ij}^\ell \int_0^1 P_k(\mu') V_{jn}^\ell(\mu') d\mu' \\ &- \frac{1}{2} \sum_{\ell} (-)^\ell \sum_{ij} P_q(\mu) U_{mi}^\ell(\mu) C_{ij}^\ell \int_0^1 \frac{\mu' \sigma_m}{\mu \sigma_n + \mu' \sigma_m} P_k(\mu') V_{jn}^\ell(\mu') d\mu'. \end{aligned}$$

On the other hand if equation (4.12a) is multiplied by  $\sigma_m P_q(\mu)$ , we find after interchanging  $k$  with  $q$  and  $\mu$  with  $\mu'$  that

$$\begin{aligned} \sigma_m P_k(\mu') V_{mn}^q(\mu') &= \sigma_m \delta_{mn} P_k(\mu') P_q(-\mu') \\ &+ \frac{1}{2} \sum_{\ell} (-)^{\ell} \sum_{ij} \int_0^1 P_q(\mu) U_{mi}^{\ell}(\mu) C_{ij}^{\ell} \frac{\mu' \sigma_m}{\mu \sigma_n + \mu' \sigma_m} P_k(\mu') V_{jn}^{\ell}(\mu') d\mu. \end{aligned}$$

These two equations are then integrated over the range (0,1), the first with respect to  $\mu$  and the second with respect to  $\mu'$ . Adding the resulting pair of equations together gives

$$\begin{aligned} \sigma_n \int_0^1 P_q(\mu) U_{mn}^k(\mu) d\mu + \sigma_m \int_0^1 P_k(\mu') V_{mn}^q(\mu') d\mu' \\ = \left[ (-)^k \sigma_n + (-)^q \sigma_m \right] \delta_{mn} \int_0^1 P_k(\mu) P_q(\mu) d\mu \\ + \frac{1}{2} \sum_{\ell} (-)^{\ell} \sum_{ij} \int_0^1 P_q(\mu) U_{mi}^{\ell}(\mu) d\mu C_{ij}^{\ell} \int_0^1 P_k(\mu') V_{jn}^{\ell}(\mu') d\mu'. \end{aligned}$$

The integral of the product of Legendre Polynomials is classical (Ryshik and Gradstein, 1963) and the last equation can be written in matrix notation as

$$\tilde{M}^{qk} \tilde{\Sigma} + \tilde{\Sigma} N^{kq} = (-)^k \delta_{kq} \frac{2}{2k+1} \tilde{\Sigma} + \frac{1}{2} \sum_{\ell} (-)^{\ell} \tilde{M}^{q\ell} \tilde{C}^{\ell} \tilde{N}^{k\ell}. \quad (A.1)$$

If we now define

$$\tilde{P}^{qk} = (-)^{q-1} \delta_{qk} I + \frac{1}{2} \tilde{M}^{qk} \tilde{\Sigma} \tilde{W}^k$$

$$\tilde{Q}^{qk} = (-)^{q-1} \delta_{qk} I + \frac{1}{2} \tilde{W}^k \tilde{\Sigma} \tilde{N}^{qk}$$

with

$$\tilde{W}^k = \tilde{\Sigma}^{-1} \tilde{C}^k \tilde{\Sigma}^{-1}$$

and

$$\tilde{D}^k = I - \frac{1}{2k+1} \tilde{W}^k \tilde{\Sigma},$$



then equation (A.1) may be written as

$$\sum_{\ell} (-)^{\ell} \tilde{P}^{q\ell} (\tilde{W}^{\ell})^{-1} \tilde{Q}^{k\ell} = (-)^k \delta_{kq} (\tilde{W}^k)^{-1} \tilde{D}^k. \quad (\text{A.2})$$

If finally from these various matrices four super-matrices

$\tilde{P}$ ,  $\tilde{Q}$ ,  $\tilde{W}$ ,  $\tilde{D}$  are constructed which may be partitioned as

$$\tilde{P} = \begin{pmatrix} \tilde{P}^{00} & \tilde{P}^{01} & \tilde{P}^{02} & \dots \\ \tilde{P}^{10} & \tilde{P}^{11} & \tilde{P}^{12} & \dots \\ \tilde{P}^{20} & \tilde{P}^{21} & \tilde{P}^{22} & \dots \end{pmatrix}$$

$$\tilde{Q} = \begin{pmatrix} \tilde{Q}^{00} & \tilde{Q}^{10} & \tilde{Q}^{20} & \dots \\ \tilde{Q}^{01} & \tilde{Q}^{11} & \tilde{Q}^{21} & \dots \\ \tilde{Q}^{02} & \tilde{Q}^{12} & \tilde{Q}^{22} & \dots \end{pmatrix}$$

$$\tilde{W} = \begin{pmatrix} \tilde{W}^0 & 0 & 0 & \dots \\ 0 & \tilde{W}' & 0 & \dots \\ 0 & 0 & \tilde{W}^2 & \dots \end{pmatrix}$$

$$\tilde{D} = \begin{pmatrix} \tilde{D}^0 & 0 & 0 & \dots \\ 0 & \tilde{D}' & 0 & \dots \\ 0 & 0 & \tilde{D}^2 & \dots \end{pmatrix}$$

then equation (A.2) may be written compactly as

$$\tilde{P} \tilde{W}^{-1} \tilde{Q} = \tilde{W}^{-1} \tilde{D}.$$

Hence

$$\underset{\sim}{W}^{-1} = \underset{\sim}{P}^{-1} \underset{\sim}{W}^{-1} \underset{\sim}{D} \underset{\sim}{Q}^{-1}$$

or by inversion

$$\underset{\sim}{Q} \underset{\sim}{D}^{-1} \underset{\sim}{W} \underset{\sim}{P} = \underset{\sim}{W}$$

and in terms of the submatrices defined earlier the last equation is

$$\sum_{\ell} (-)^{\ell} \underset{\sim}{Q}^{\ell k} (\underset{\sim}{D}^{\ell})^{-1} \underset{\sim}{W}^{\ell} \underset{\sim}{P}^{\ell q} = (-)^q \delta_{qk} \underset{\sim}{W}^q. \quad (\text{A.3})$$

If we restrict ourselves to the one group problem with total cross section unity, all these matrices collapse to scalars involving the  $\phi_{\ell}(\mu)$  functions of Busbridge (1960) so that

$$\underset{\sim}{P}^{kq} \rightarrow p_{kq} = (-)^{q-1} \delta_{qk} + \frac{2k+1}{2} \omega^k \int_0^1 p_q(\mu) \phi_k(\mu) d\mu$$

$$\underset{\sim}{Q}^{kq} \rightarrow p_{kq}$$

$$\underset{\sim}{W}^k \rightarrow \omega_k = (2k+1) \sigma^k$$

$$\underset{\sim}{D}^k \rightarrow d_k = 1 - \frac{\omega_k}{2k+1}$$

and we recover the relations between the coefficients  $p_{kq}$  established by Busbridge.

## A.2 Connections between the Matrices $U^\ell(\mu)$ and $V^\ell(\mu)$

That this much of Busbridge's analysis generalises so readily to the multigroup case suggests that more of it may. In particular it suggests that there may for the multigroup case be an analogy to the result that the  $\phi_\ell(\mu)$  functions are polynomials in  $\mu$  multiplied by a single H-function. This possibility is now explored briefly.

From equation (4.11a) we find that

$$\begin{aligned}
 & (k+1)\sigma_m U_{mn}^{k+1}(\mu) + (2k+1)\sigma_n \mu U_{mn}^k(\mu) + k\sigma_m U_{mn}^{k-1}(\mu) \\
 & = \delta_{mn} [(k+1)\sigma_m P_{k+1}(-\mu) + (2k+1)\sigma_n \mu P_k(-\mu) + k\sigma_m P_{k-1}(\mu)] \\
 & + \frac{\mu}{2} \sum_{\ell} (-)^{\ell} \sum_{ij} U_{mi}^{\ell}(\mu) C_{ij}^{\ell} \int_0^1 V_{jn}^{\ell}(\mu') \times A \, d\mu' \quad (A.4)
 \end{aligned}$$

where

$$\begin{aligned}
 A & \equiv \frac{(k+1)\sigma_m P_{k+1}(\mu') + (2k+1)\sigma_n \mu P_k(\mu') + k\sigma_m P_{k-1}(\mu')}{\mu\sigma_m + \mu'\sigma_m} \\
 & = (2k+1)P_k(\mu')
 \end{aligned}$$

because of the relations

$$\begin{aligned}
 & (k+1)P_{k+1}(-\mu) + (2k+1)\mu P_k(-\mu) + kP_{k-1}(-\mu) = 0 \quad (A.5) \\
 & P_k(-\mu) = (-)^k P_k(\mu)
 \end{aligned}$$

existing between the Legendre polynomials. When  $m$  and  $n$  are

unequal the Kronecker delta in the first term on the right hand side of equation (A.4) causes this term to vanish, and when  $m$  and  $n$  are equal this term vanishes because of equation (A.5). Equation (A.4) becomes then

$$\begin{aligned} & (k+1)\sigma_m U_{mn}^{k+1}(\mu) + (2k+1)\sigma_n \mu U_{mn}^k(\mu) + k\sigma_m U_{mn}^{k-1}(\mu) \\ &= \frac{\mu}{2} \sum_{\ell} (-)^{\ell} \sum_{ij} U_{mn}^{\ell}(\mu) C_{ij}^{\ell} \int_0^1 V_{jn}^{\ell}(\mu') (2k+1) P_k(\mu') d\mu' \end{aligned}$$

or in matrix notation

$$\begin{aligned} & (k+1) \underline{\Sigma} \underline{U}^{k+1}(\mu) + (2k+1) \mu \underline{U}^k(\mu) \underline{\Sigma} + k \underline{\Sigma} \underline{U}^{k-1}(\mu) \\ &= \frac{2k+1}{2} \mu \sum_{\ell} (-)^{\ell} \underline{U}^{\ell}(\mu) \underline{C}^{\ell} \underline{N}^{k\ell}. \end{aligned}$$

Elementary matrix manipulations then reduce this to the simpler form

$$\begin{aligned} & \frac{1}{2k+1} \underline{\Sigma} \{ (k+1) \underline{U}^{k+1}(\mu) + k \underline{U}^{k-1}(\mu) \} \\ &= \mu \sum_{\ell=0}^L (-)^{\ell} \underline{U}^{\ell}(\mu) \underline{\Sigma} \underline{Q}^{k\ell}. \end{aligned} \quad (A.6)$$

Beginning with equation (4.12a) and following through a similar analysis we are led to the companion equation

$$\begin{aligned} & \frac{1}{2k+1} \{ (k+1) \underline{V}^{k+1}(\mu) + k \underline{V}^{k-1}(\mu) \} \\ &= \mu \sum_{\ell=0}^L (-)^{\ell} \underline{P}^{k\ell} \underline{\Sigma} \underline{V}^{\ell}(\mu) \end{aligned} \quad (A.7)$$

and both equations (A.6) (A.7) are restricted to the range of values  $k = 0, 1, 2, \dots, L-1$ .

In the one group problem with unit total cross section equations (A.6), (A.7) collapse to a single equation in the  $\phi_\ell(\mu)$  function

$$\frac{1}{2k+1} \{ (k+1) \phi_{k+1}(\mu) + k \phi_{k-1}(\mu) \} = \mu \sum_{\ell} (-)^{\ell} p_{k\ell} \phi_{\ell}(\mu)$$

from which Busbridge (1960) deduced that the  $\phi_{\ell}(\mu)$  are each equal to a polynomial  $q_{\ell}(\mu)$  multiplied by a single function  $H(\mu)$  determined by the anisotropic scattering coefficients.

In the multigroup problem, equations (A.6), (A.7) show that the elements of the various matrices  $\tilde{U}^{\ell}(\mu)$  are connected by homogeneous algebraic equations, and that the same holds true for the matrices  $\tilde{V}^{\ell}(\mu)$ . The form of the equations suggests, however, that this interrelationship will not be expressible by writing each  $\tilde{U}^{\ell}(\mu)$  or  $\tilde{V}^{\ell}(\mu)$  as a simple product of a polynomial matrix with some other matrices independent of  $\ell$ . It thus seems unlikely that this part of Busbridge's analysis of anisotropic scattering problems can be generalised for multigroup theory.

### A.3 Moments for Isotropic Scattering

If all scattering is treated as isotropic in the laboratory system, then the sum over  $\ell$  in equation (4.1) contains only the  $\ell = 0$  term. We need then only consider the single pair

of matrices  $\tilde{U}(\mu), \tilde{V}(\mu)$  (dropping the superscript zero) discussed by Pahor and Shultis (1969). These matrices satisfy

$$\tilde{U}(\mu) = \tilde{I} + \frac{\mu}{2} \int_0^1 A(\mu, \mu') * [\tilde{U}(\mu) \tilde{C} \tilde{V}(\mu')] d\mu' \quad (\text{A.8})$$

$$\tilde{V}(\mu) = \tilde{I} + \frac{\mu}{2} \int_0^1 A(\mu', \mu) * [\tilde{U}(\mu') \tilde{C} \tilde{V}(\mu)] d\mu' \quad (\text{A.9})$$

where  $\tilde{C}$  has been written for the isotropic transfer matrix  $\tilde{C}^0$ .

It is possible to derive a set of moment relationships somewhat different to those of Section A.1. With the definitions

$$\tilde{M}^q = \int_0^1 \mu^q \tilde{U}(\mu) d\mu$$

$$\tilde{N}^q = \int_0^1 \mu^q \tilde{V}(\mu) d\mu$$

these relationships can be computed by post multiplying equation (A.8) by  $\mu^q(\Sigma)^{q+1}$  and integrating the result with respect to  $\mu$  over the range (0,1). The (m,n) element of the resulting matrix equation is

$$\begin{aligned}
\sigma_n^{q+1} M_{mn}^q &= \frac{\sigma_n^{q+1}}{q+1} \delta_{mn} = \frac{1}{2} \sum_{ij} \int_0^1 (\sigma_n \mu)^{q+1} U_{mi}(\mu) d\mu C_{ij} \int_0^1 \frac{V_{jn}(\mu')}{\mu \sigma_n + \mu' \sigma_m} d\mu' \\
&= \frac{\sigma_n^{q+1}}{q+1} \delta_{mn} + \frac{1}{2} \sum_{ij} \sum_{k=0}^q (-)^k \int_0^1 (\sigma_n \mu)^{q-k} U_{mi}(\mu) d\mu C_{ij} \int_0^1 (\sigma_m \mu')^k V_{jn}(\mu') d\mu' \\
&+ \frac{1}{2} (-)^{q+1} \sum_{ij} \int_0^1 U_{mi}(\mu) d\mu C_{ij} \int_0^1 \frac{(\sigma_m \mu')^{q+1}}{\mu \sigma_n + \mu' \sigma_m} V_{jn}(\mu') d\mu'.
\end{aligned}$$

On the other hand the  $(m,n)$  element of the equation derived by premultiplication of equation (A.9) by  $\mu^q(\Sigma)^{q+1}$  and integration with respect to  $\mu$  is

$$\sigma_m^{q+1} N_{mn}^q = \frac{\sigma_m^{q+1}}{q+1} \delta_{mn} + \frac{1}{2} \sum_{ij} \int_0^1 \frac{U_{mi}(\mu')}{\mu' \sigma_n + \mu \sigma_m} d\mu' C_{ij} \int_0^1 (\sigma_m \mu)^{q+1} V_{jn}(\mu) d\mu.$$

From these last two equations and the definitions of  $\underline{M}^q$  and  $\underline{N}^q$  it follows immediately that

$$\begin{aligned}
\sigma_n^{q+1} M_{mn}^q + (-)^q \sigma_m^{q+1} N_{mn}^q &= \frac{\delta_{mn}}{q+1} (\sigma_n^{q+1} + (-)^q \sigma_m^{q+1}) \\
&+ \frac{1}{2} \sum_{k=0}^q (-)^k \sum_{ij} \sigma_n^{q-k} M_{mi}^{q-k} C_{ij} \sigma_m^k N_{jn}^k
\end{aligned}$$

or in matrix notation

$$\begin{aligned}
\underline{M}^q(\Sigma)^{q+1} + (-)^q \underline{N}^q(\Sigma)^{q+1} &= \frac{1+(-)^q}{q+1} (\Sigma)^{q+1} \\
&+ \frac{1}{2} \sum_{k=0}^q (-)^k (\Sigma)^k \underline{M}^{q-k} \underline{C}^k \underline{N}^k (\Sigma)^{q-k}.
\end{aligned} \tag{A.10}$$

The moment relationship (A.10) has been established for  $q = 0, 1, 2, \dots$ . It is interesting to note that it remains true for  $q = -1$  in the sense that, if the sum  $\sum_{k=0}^{-1}$  is interpreted as being zero, the relationship takes the form

$$\tilde{M}^{-1} - \tilde{N}^{-1} = 0$$

or

$$\int_0^1 \tilde{U}(\mu) \frac{d\mu}{\mu} - \int_0^1 \tilde{V}(\mu) \frac{d\mu}{\mu} = 0.$$

Now both these integrals diverge but from equations (A.8), (A.9) it is easy to show that

$$\int_0^1 [\tilde{U}(\mu) - \tilde{V}(\mu)] \frac{d\mu}{\mu} = 0$$

which is the required interpretation of (A.10).